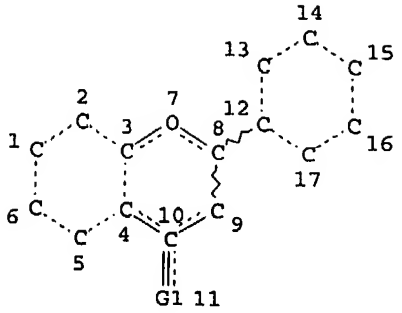
=> d que 129
L1 STR



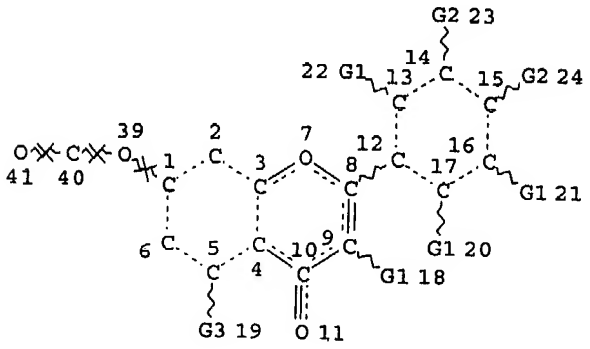
$X = O$

$R_{10} + R_{11}$ or $R_{11} + R_{12} = -O-C-O-$

VAR G1=O/S
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L2 36287 SEA FILE=REGISTRY SSS FUL L1
L3 STR



Ak @25 NH~Me @26 27

Ak~COOH @28 29 O=C~NH 30 @31 32 O=C~O~Ak 33 @34 35 36 S~Me @37 38

VAR G1=H/F
VAR G2=H/O/SH/X/25/NH2/26/CN/COOH/28/31/34/CF3
VAR G3=OH/NH2/26/SH/37
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 25
CONNECT IS E2 RC AT 28
CONNECT IS E1 RC AT 36
CONNECT IS E2 RC AT 37
DEFAULT MLEVEL IS ATOM

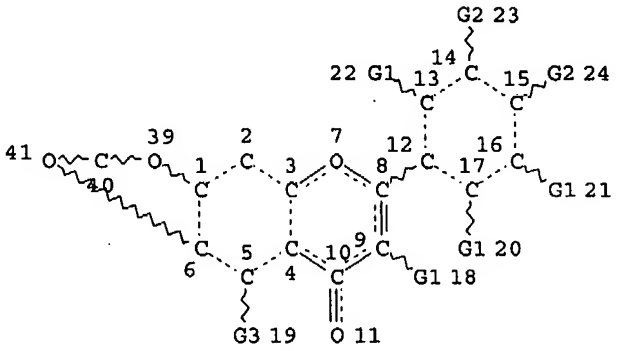
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 41

STEREO ATTRIBUTES: NONE
L6 1066 SEA FILE=REGISTRY SUB=L2 SSS FUL L3
L11 STR

Ak @25 NH~Me @26 27 Ak~COOH @28 29 O=C~NH 30 @31 32 O=C~O~Ak 33 @34 35 36

S~Me
@37 38



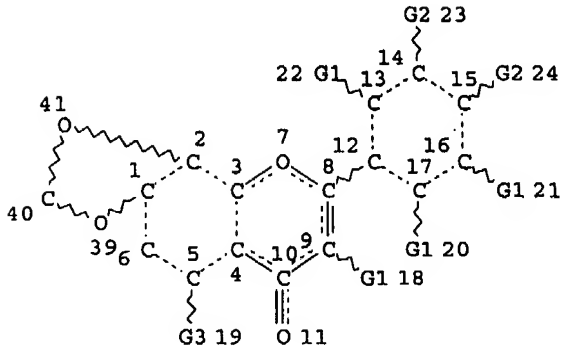
VAR G1=H/F
VAR G2=H/O/SH/X/25/NH2/26/CN/COOH/28/31/34/CF3
VAR G3=OH/NH2/26/SH/37
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 25
CONNECT IS E2 RC AT 28
CONNECT IS E1 RC AT 36
CONNECT IS E2 RC AT 37
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 41

STEREO ATTRIBUTES: NONE
L12 6 SEA FILE=REGISTRY SUB=L2 SSS FUL L11
L13 STR

Ak @25 NH~Me @26 27 Ak~COOH @28 29 O=C~NH 30 @31 32 O=C~O~Ak 33 @34 35 36

S~Me @37 38



VAR G1=H/F
VAR G2=H/O/SH/X/25/NH2/26/CN/COOH/28/31/34/CF3
VAR G3=OH/NH2/26/SH/37
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 25
CONNECT IS E2 RC AT 28
CONNECT IS E1 RC AT 36
CONNECT IS E2 RC AT 37
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 41

STEREO ATTRIBUTES: NONE
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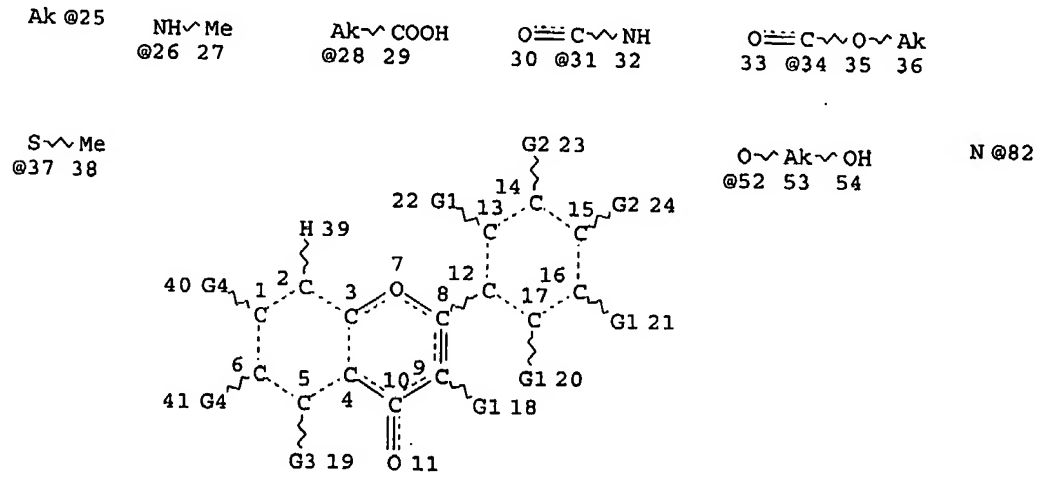
L15 7 SEA FILE=REGISTRY ABB=ON PLU=ON L12 OR L14
L22 STR



Page 1-A

Page 2-A

VAR G1=H/F
VAR G2=H/O/SH/X/25/NH2/26/CN/COOH/28/31/34/CF3
VAR G3=OH/NH2/26/SH/37
VAR G4=H/OH/X/25/NH2/CN/COOH/28/31/34/52/CF3/55/57/60/63/66/68/71/75
VAR G5=82/83/85/87
NODE ATTRIBUTES:
NSPEC IS RC AT 82
NSPEC IS RC AT 84
NSPEC IS RC AT 86
NSPEC IS RC AT 89
CONNECT IS E1 RC AT 25
CONNECT IS E2 RC AT 28
CONNECT IS E1 RC AT 36
CONNECT IS E2 RC AT 37
CONNECT IS E1 RC AT 56
CONNECT IS E1 RC AT 65

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CONNECT IS E1  RC AT  78
CONNECT IS E1  RC AT  79
CONNECT IS E2  RC AT  83
CONNECT IS E2  RC AT  88
DEFAULT MLEVEL IS ATOM
GGCAT   IS SAT  AT  67
GGCAT   IS SAT  AT  70
GGCAT   IS LIN  SAT  AT  83
GGCAT   IS MCY  UNS  AT  85
GGCAT   IS MCY  UNS  AT  87
GGCAT   IS LIN  SAT  AT  88
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M4-X5 C  E1 O  AT  67
ECOUNT  IS M4-X5 C  E1 O  AT  70
ECOUNT  IS E6 C  AT  85
ECOUNT  IS E6 C  AT  87

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  79

STEREO ATTRIBUTES: NONE
L23        1475 SEA FILE=REGISTRY SUB=L2 SSS FUL L22
L27          24 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L15
L28           9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND L15
L29          24 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L27 OR L28


=> d l29 ibib ab hitstr 1-24

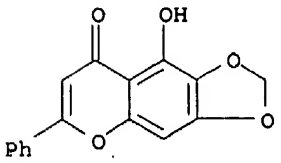
L29  ANSWER 1 OF 24  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2004:971408  HCAPLUS
DOCUMENT NUMBER:          142:130223
TITLE:                    A photoaffinity probe designed for host-specific
                          signal flavonoid receptors in phytopathogenic
                          Peronosporomycete zoospores of Aphanomyces cochlioides
AUTHOR(S):                Sakihama, Yasuko; Shimai, Takashi; Sakasai,
                          Mitsuyoshi; Ito, Toshiaki; Fukushi, Yukiharu;
                          Hashidoko, Yasuyuki; Tahara, Satoshi
CORPORATE SOURCE:         Laboratory of Ecological Chemistry, Graduate School of
                          Agriculture, Hokkaido University, Kita-ku, Sapporo,
                          060-8589, Japan
SOURCE:                   Archives of Biochemistry and Biophysics (2004),
                          432(2), 145-151
                          CODEN: ABBIA4; ISSN: 0003-9861
PUBLISHER:                Elsevier
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   Aphanomyces cochlioides zoospores show chemotaxis to cochliophilin A
     (5-hydroxy-6,7-methylenedioxyflavone, 1), a host derived attractant, and
     also respond to 5,7-dihydroxyflavone (2) known as an equivalent
     chemoattractant.  To investigate the chemotactic receptors in the
     zoospores, we designed photoaffinity probes 4'-azido-5,7-dihydroxyflavone
     (3) and 4'-azido-7-O-biotinyl-5-hydroxyflavone (4) considering chemical
     structure of 2.  Both 3 and 4 had zoospore attractant activity which was
     competitive with that of 1.  When zoospores were treated with the
     biotinylated photoaffinity probe followed by UV irradiation and
     streptavidin-gold or peroxidase-conjugated streptavidin, probe-labeled
     proteins were detected on the cell membrane.  This result indicated that
```

the 1-specific-binding proteins, a candidate for hypothetical cochliophilin A receptor, were localized on the cell membrane of the zoospores. This is the first exptl. evidence of flavonoid-binding proteins being present in zoospores, using chemical synthesized azidoflavone as photoaffinity-labeling reagent.

IT **110204-45-0**, Cochliophilin A
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(photoaffinity probe designed for host-specific signal flavonoid receptors in phytopathogenic Peronosporomycete zoospores of Aphanomyces cochlioides)

RN 110204-45-0 HCAPLUS

CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 2 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:770227 HCAPLUS

DOCUMENT NUMBER: 141:405646

TITLE: Increased Anti-P-glycoprotein Activity of Baicalein by Alkylation on the A Ring

AUTHOR(S): Lee, Yashang; Yeo, Hosup; Liu, Shwu-Huey; Jiang, Zaoli; Savizky, Ruben M.; Austin, David J.; Cheng, Yung-chi

CORPORATE SOURCE: Department of Pharmacology, Yale University School of Medicine, New Haven, CT, 06520, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(22), 5555-5566
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

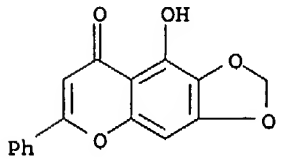
LANGUAGE: English

AB The aqueous extract of Scutellariae baicalensis Georgi has inhibitory activity against P-gp 170, a multiple drug resistant gene product. Baicalein, one of the major flavones, was found to be responsible for this activity. The hydroxyl groups of the A ring of baicalein were systematically alkylated in order to assess the effect of such modifications on the activity against P-gp 170. The impact of the baicalein modifications on activity against the growth of a human nasopharyngeal cancer cell line KB and its P-gp 170 overexpressing cell line KB/MDR were also examined The results indicate that alkylation of R5 of baicalein does not have a major impact on the interaction with P-gp 170, whereas alkylation of R6 or R7 alone or both, could enhance the interaction of baicalein with P-gp 170 as well as the amount of intracellular accumulation of vinblastine, a surrogate marker for the activity of P-gp 170 pump of KB/MDR cells. In this case, the optimal linear alkyl functionality is a Pr side chain. These modifications could also alter the activity of compds. inhibiting cell growth. Among the different compds. synthesized, the most potent mol. against P-gp 170 is 5-methoxy-6,7-dipropyloxyflavone. Its inhibitory

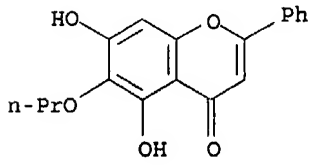
activity against P-gp 170 is approx. 40 times better, based on EC50 (concentration of the compound enhancing 50% of the intracellular vinblastine accumulation in the KB/MDR cells) and 3 times higher, based on Amax (the intracellular vinblastine accumulation of the KB/MDR cells caused by the compound) as compared to baicalein. One compound is also a more selective inhibitor than baicalein against P-gp 170, because its cytotoxicity is less than that observed for baicalein. The growth inhibitory IC50 of the compound against KB and KB/MDR cells are about the same, suggesting that compound 23 is unlikely to be a substrate of P-gp 170 pump. Acetylation of R6, R7 or both could also decrease EC50 and increase Amax. Acetylated compds. are more toxic than baicalein, and their potency against cell growth is compromised by the presence of P-gp 170, suggesting that these compds. are substrates of P-gp 170. Benzylation of R6 or R7 but not both also enhanced anti-P-gp170 activity and potency against cell growth; however, the presence of P-gp 170 in cells did not have an impact on their sensitivity to these mols., suggesting that the benzylated compds. are inhibitors but not substrates of P-gp 170, and perhaps have a different mechanism of action. In conclusion, the substitutions of R6 and R7 hydroxyl groups by alkoxy groups, acetoxy groups, or benzyloxy groups could yield compds. with different modes of action against P-gp 170 with different mechanisms of action against cell growth.

IT **110204-45-0P**, 5-Hydroxy-6,7-(methylenedioxy)flavone
792923-65-0P 792923-66-1P 792923-71-8P
792923-72-9P 792923-75-2P 792923-77-4P
792923-80-9P
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(increased anti-P-glycoprotein activity of baicalein by alkylation on A ring)

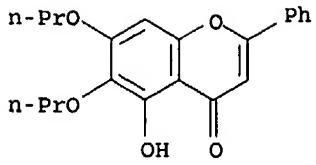
RN 110204-45-0 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



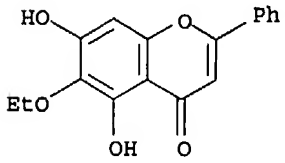
RN 792923-65-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-phenyl-6-propoxy- (9CI) (CA INDEX NAME)



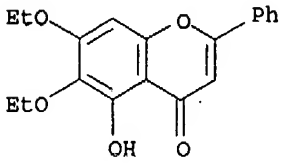
RN 792923-66-1 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-2-phenyl-6,7-dipropoxy- (9CI) (CA INDEX NAME)



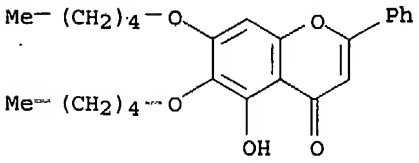
RN 792923-71-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 6-ethoxy-5,7-dihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



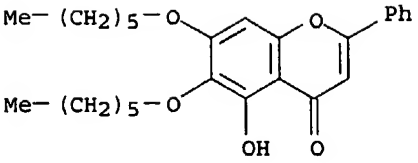
RN 792923-72-9 HCAPLUS
CN 4H-1-Benzopyran-4-one, 6,7-diethoxy-5-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



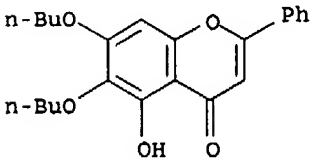
RN 792923-75-2 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-6,7-bis(pentyloxy)-2-phenyl- (9CI) (CA INDEX NAME)



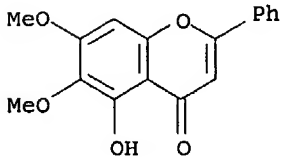
RN 792923-77-4 HCAPLUS
CN 4H-1-Benzopyran-4-one, 6,7-bis(hexyloxy)-5-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



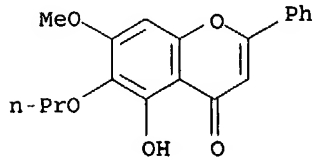
RN 792923-80-9 HCAPLUS
CN 4H-1-Benzopyran-4-one, 6,7-dibutoxy-5-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



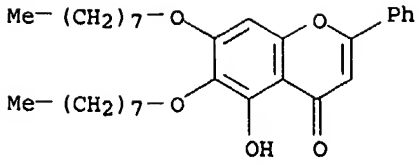
IT **740-33-0P**, 5-Hydroxy-6,7-dimethoxyflavone **792923-67-2P**
792923-73-0P 792923-74-1P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(increased anti-P-glycoprotein activity of baicalein by alkylation on A ring)
RN 740-33-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-6,7-dimethoxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 792923-67-2 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-7-methoxy-2-phenyl-6-propoxy- (9CI) (CA INDEX NAME)



RN 792923-73-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-6,7-bis(octyloxy)-2-phenyl- (9CI) (CA INDEX NAME)



RN 792923-74-1 HCAPLUS
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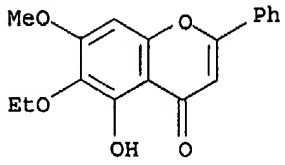
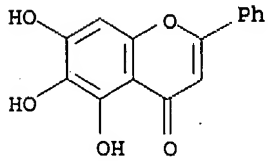


IT **491-67-8**, Baicalein
RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(increased anti-P-glycoprotein activity of baicalein by alkylation on A ring)
RN 491-67-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 3 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:433756 HCAPLUS
DOCUMENT NUMBER: 140:417945
TITLE: 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use
INVENTOR(S): Lahey, Thomas; Rajadhyaksha, Vithal J.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 19 pp., Cont.-in-part of U.S. Pat. Appl. 2003 69,192.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004102386	A1	20040527	US 2003-652624	20030829

US 2003069192	A1	20030410	US 2002-236861	20020906
US 6774142	B2	20040810		
US 2004209825	A1	20041021	US 2004-838766	20040504
WO 2005020981	A1	20050310	WO 2004-US28244	20040830

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:	US 2001-317666P	P 20010906
	US 2002-407125P	P 20020830
	US 2002-236861	A2 20020906
	US 2003-652624	A 20030829

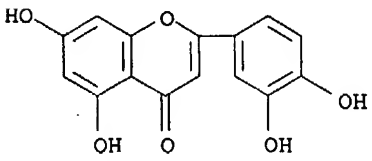
OTHER SOURCE(S): MARPAT 140:417945

AB The invention discloses 3-deoxyflavonoid compds. and methods for inhibiting T-cell activity and treating diseases and disorders (e.g. autoimmune disorders, inflammatory disorders, diabetes, ALS, MS, rheumatoid arthritis, etc.). In some cases the efficacy and/or duration of action of luteolin and/or other 3-deoxyflavonoid compds. may be increased by administering such compds. along with rutin, a rutin congener and/or a rutin derivative Also, in some cases, first pass metabolism of luteolin or other 3-deoxyflavonoids may be avoided by administering such compds. by parenteral routes (e.g., routes wherein absorption occurs at sites other than the stomach or intestinal mucosa, such as sublingual, buccal, intranasal, injection, etc.).

IT **491-70-3**, Luteolin **501445-13-2 501445-14-3 501445-15-4 501445-16-5 501445-18-7 501445-19-8**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

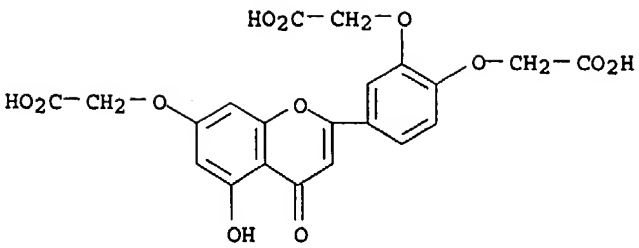
RN 491-70-3 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

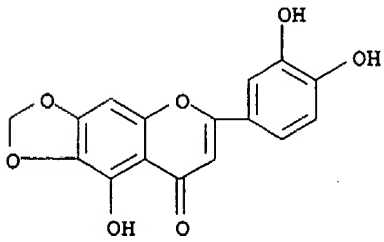


RN 501445-13-2 HCAPLUS

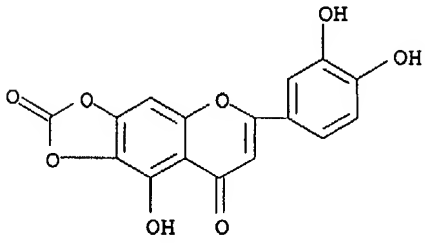
CN Acetic acid, 2,2'-[[4-[7-(carboxymethoxy)-5-hydroxy-4-oxo-4H-1-benzopyran-2-yl]-1,2-phenylene]bis(oxy)]bis- (9CI) (CA INDEX NAME)



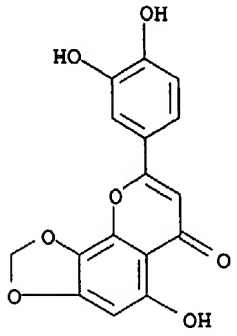
RN 501445-14-3 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 6-(3,4-dihydroxyphenyl)-9-hydroxy- (9CI) (CA INDEX NAME)



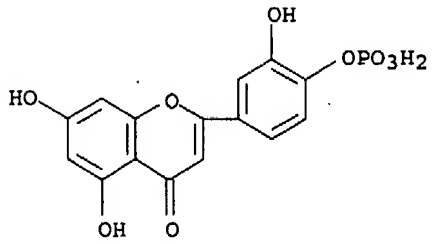
RN 501445-15-4 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-2,8-dione, 6-(3,4-dihydroxyphenyl)-9-hydroxy- (9CI) (CA INDEX NAME)



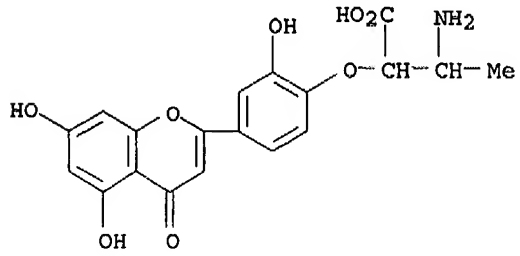
RN 501445-16-5 HCAPLUS
CN 6H-1,3-Dioxolo[4,5-h][1]benzopyran-6-one, 8-(3,4-dihydroxyphenyl)-5-hydroxy- (9CI) (CA INDEX NAME)



RN 501445-18-7 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-[3-hydroxy-4-(phosphonooxy)phenyl]-(9CI) (CA INDEX NAME)



RN 501445-19-8 HCAPLUS
CN Butanoic acid, 3-amino-2-[4-(5,7-dihydroxy-4-oxo-4H-1-benzopyran-2-yl)-2-hydroxyphenoxy]- (9CI) (CA INDEX NAME)



L29 ANSWER 4 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:368882 HCAPLUS
DOCUMENT NUMBER: 140:375072
TITLE: Preparation of chromone derivatives for treatment of septic shock, organ injury, and other disorders
INVENTOR(S): Yen, Mao-Hsiung; Wu, Edwin S. C.
PATENT ASSIGNEE(S): Jenken Biosciences, Inc., USA
SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037193	A2	20040506	WO 2003-US33578	20031022
WO 2004037193	A3	20050217		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

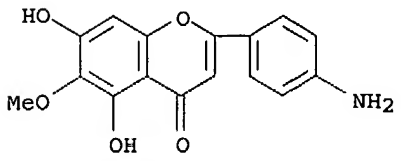
CA 2421887	AA	20040422	CA 2003-2421887		20030313
PRIORITY APPLN. INFO.:			US 2002-420306P	P	20021022
			US 2003-453771P	P	20030311

OTHER SOURCE(S): MARPAT 140:375072

AB The title compds. I [wherein R1-R3 = independently H, alkyl, alkenyl, alkynyl, SO3H, PO3H2, carbohydrate, etc.; X1 and X2 = independently Ar-X3-T; Ar = none, Ph, furanyl, thienyl, pyridyl, cyclohexyl, or PhCH2; X3 = H, C, N, O, S, etc.; with provisos] or pharmaceutically acceptable salts thereof are prepared For example, the compound II was prepared in a multi-step synthesis. I are useful for the prevention and treatment of septic shock, organ injury, and other disorders (no data).

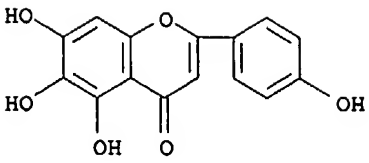
IT **16297-04-4P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of chromone derivs. for treatment of septic shock, organ injury, and other disorders)

RN 16297-04-4 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2-(4-aminophenyl)-5,7-dihydroxy-6-methoxy- (9CI) (CA INDEX NAME)

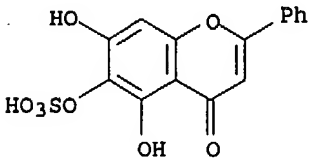


IT **529-53-3P 23608-41-5P 63934-55-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of chromone derivs. for treatment of septic shock, organ injury, and other disorders)

RN 529-53-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

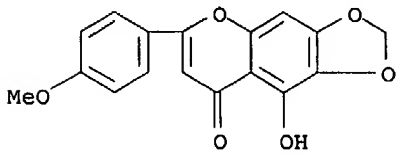


RN 23608-41-5 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-phenyl-6-(sulfooxy)-, monosodium salt (9CI) (CA INDEX NAME)



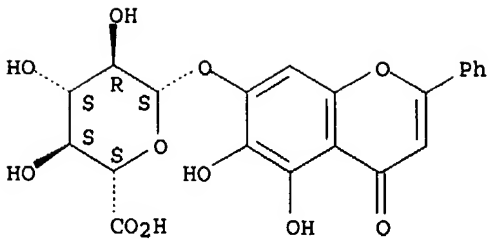
● Na

RN 63934-55-4 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

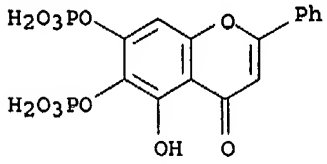


IT **21967-41-9**, Baicalin **23608-39-1 23615-79-4**
23688-74-6 23688-76-8 47363-04-2
47363-07-5 685143-80-0 685143-81-1
685143-83-3 685143-84-4 685143-85-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(drug containing; preparation of chromone derivs. for treatment of septic shock,
organ injury, and other disorders)
RN 21967-41-9 HCAPLUS
CN β-D-Glucopyranosiduronic acid, 5,6-dihydroxy-4-oxo-2-phenyl-4H-1-benzopyran-7-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

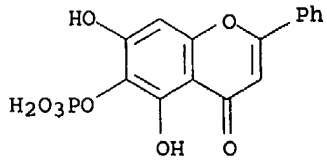


RN 23608-39-1 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-2-phenyl-6,7-bis(phosphonooxy)-, tetrapotassium salt (9CI) (CA INDEX NAME)



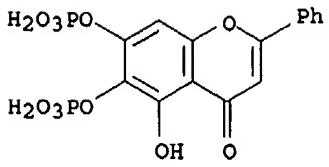
●4 K

RN 23615-79-4 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-phenyl-6-(phosphonooxy)-, disodium salt (9CI) (CA INDEX NAME)



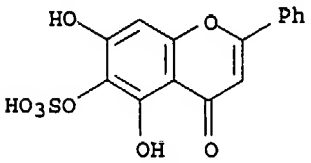
●2 Na

RN 23688-74-6 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-2-phenyl-6,7-bis(phosphonooxy)-, tetrasodium salt (9CI) (CA INDEX NAME)



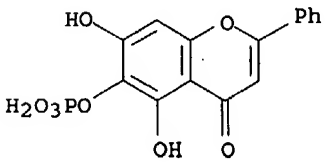
●4 Na

RN 23688-76-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-phenyl-6-(sulfooxy)-, monopotassium salt (9CI) (CA INDEX NAME)

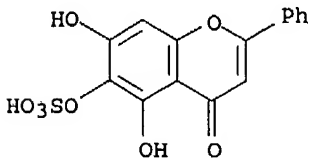


● K

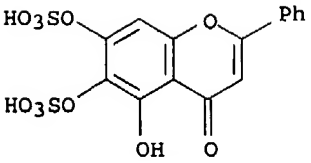
RN 47363-04-2 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-phenyl-6-(phosphonooxy)- (9CI) (CA INDEX NAME)



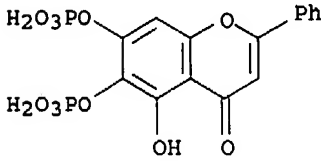
RN 47363-07-5 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-phenyl-6-(sulfooxy)- (9CI) (CA INDEX NAME)



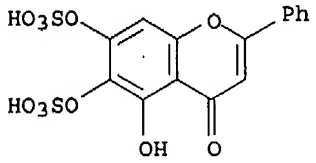
RN 685143-80-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-2-phenyl-6,7-bis(sulfooxy)- (9CI) (CA INDEX NAME)



RN 685143-81-1 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-2-phenyl-6,7-bis(phosphonooxy)- (9CI) (CA INDEX NAME)

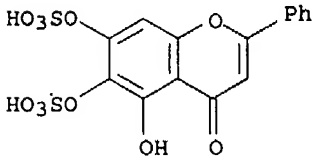


RN 685143-83-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-2-phenyl-6,7-bis(sulfooxy)-, disodium salt (9CI) (CA INDEX NAME)



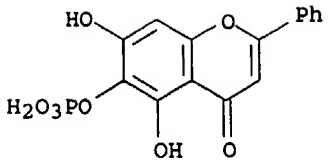
●2 Na

RN 685143-84-4 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-2-phenyl-6,7-bis(sulfooxy)-, dipotassium salt (9CI) (CA INDEX NAME)



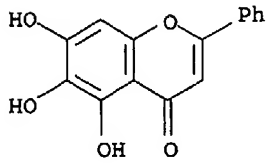
●2 K

RN 685143-85-5 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-phenyl-6-(phosphonooxy)-, dipotassium salt (9CI) (CA INDEX NAME)

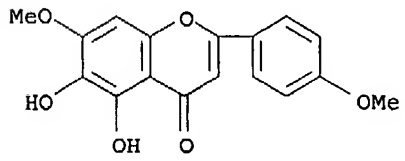


●2 K

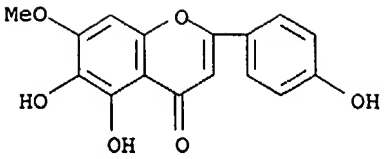
IT **491-67-8**, Baicalein
RL: RCT (Reactant); RACT (Reactant or reagent)
(drug containing; preparation of chromone derivs. for treatment of septic shock,
organ injury, and other disorders)
RN 491-67-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



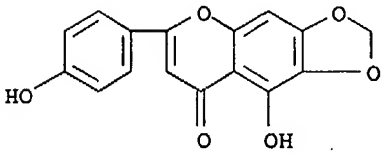
IT **10176-71-3P 23130-22-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of chromone derivs. for treatment of septic shock, organ injury, and other disorders)
RN 10176-71-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6-dihydroxy-7-methoxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 23130-22-5 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6-dihydroxy-2-(4-hydroxyphenyl)-7-methoxy- (9CI) (CA INDEX NAME)

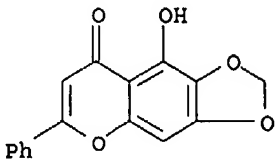


IT **60948-17-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of chromone derivs. for treatment of septic shock, organ injury, and other disorders)
RN 60948-17-6 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L29 ANSWER 5 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:276492 HCAPLUS
DOCUMENT NUMBER: 141:136744
TITLE: Interruption of the homing events of phytopathogenic Aphanomyces cochlioides zoospores by secondary metabolites from nonhost Amaranthus gangeticus
AUTHOR(S): Islam, Md. Tofazzal; Hashidoko, Yasuyuki; Ito, Toshiaki; Tahara, Satoshi
CORPORATE SOURCE: Laboratory of Ecological Chemistry, Graduate School of Agriculture, Hokkaido University, Sapporo, 060-8589, Japan
SOURCE: Journal of Pesticide Science (Tokyo, Japan) (2004), 29(1), 6-14
CODEN: JPSTCF
PUBLISHER: Pesticide Science Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB On the screening of 200 nonhost plants, an Amaranthus gangeticus extract was found to attract and subsequently inhibit the motility of Aphanomyces cochlioides zoospores. The attractant was identified as N-trans-feruloyl-4-O-methyldopamine (I) and the motility inhibitor as nicotinamide (II) using bioassay-guided fractionation and spectroscopic methods. Also isolated were cochliophilin A and chondrillasterol 3-O-β-D-glucopyranoside. I had no inhibitory effect on zoospore motility whereas II immediately halted the motility and caused encystment in a dose-dependent manner (MIC, 5 + 10-8 M). The cystospores produced by II regenerated zoospores instead of germinating. Concomitant application of I and II produced cystospores that germinated to give hyphae. TLC examns. revealed that A. gangeticus seedling exuded sufficient amts. of II from the roots. Exudation of II from A. gangeticus might be involved in its resistance against the soilborne oomycete phytopathogen A. cochlioides.
IT **110204-45-0P**, Cochliophilin A

RL: PUR (Purification or recovery); PREP (Preparation)
(of secondary metabolites from Amaranthus gangeticus)
RN 110204-45-0 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 6 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:809009 HCAPLUS
DOCUMENT NUMBER: 141:36073
TITLE: Host-specific plant signal and G-protein activator, mastoparan, trigger differentiation of zoospores of the phytopathogenic oomycete Aphanomyces cochlioides
AUTHOR(S): Islam, Md. Tofazzal; Ito, Toshiaki; Tahara, Satoshi
CORPORATE SOURCE: Graduate School of Agriculture, Division of Applied Bioscience, Laboratory of Ecological Chemistry, Hokkaido University, Kita-ku, Sapporo, 060-8589, Japan
SOURCE: Plant and Soil (2003), 255(1), 131-142
CODEN: PLSOA2; ISSN: 0032-079X
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We found that a gradient of a host-specific attractant, cochliophilin A (5-hydroxy-6,7-methylenedioxyflavone) isolated from the roots of spinach triggered encystment followed by germination of zoospores of Aphanomyces cochlioides at a concentration less than micromolar order. This compound did not affect the growth and reproduction of this phytopathogen up to 10-6 M concentration in the culture medium. We also observed that mastoparan, an activator of heterotrimeric G-protein could inhibit the motility of zoospores and then strikingly effect encystment followed by 60-80% germination of cysts. Concomitant application of cochliophilin A and mastoparan showed stronger encystment followed by 100% germination of cysts. In addition, we have observed that chems. interfering with phospholipase C activity (neomycin) and Ca2+ influx/release (EGTA and loperamide) suppress cochliophilin A or mastoparan induced encystment and germination. These results suggest that G-protein mediated signal transduction mechanism may be involved in the differentiation of the A. cochlioides zoospores. This is the first report on the differentiation of oomycete zoospores initiated by a host-specific plant signal or a G-protein activator.
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 7 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:221804 HCAPLUS
DOCUMENT NUMBER: 138:231731

TITLE: 3-Deoxyflavonoids that inhibit T-lymphocyte activation and use in treating immune disorders and inflammatory disorders
INVENTOR(S): Lahey, Thomas P.; Rajadhyaksha, V. J.
PATENT ASSIGNEE(S): Synorx, Inc., USA
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

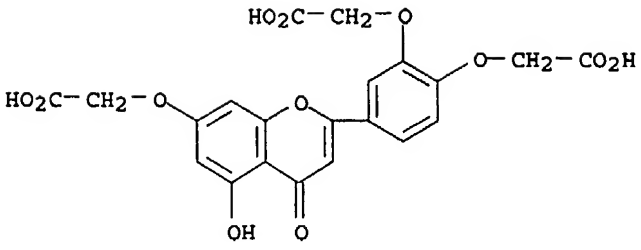
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003022994	A2	20030320	WO 2002-US28348	20020906
WO 2003022994	A3	20031009		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1429750	A2	20040623	EP 2002-798140	20020906
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002012354	A	20041130	BR 2002-12354	20020906
JP 2005504796	T2	20050217	JP 2003-527059	20020906
PRIORITY APPLN. INFO.:			US 2001-317666P	P 20010906
			US 2002-407125P	P 20020830
			WO 2002-US28348	W 20020906

OTHER SOURCE(S): MARPAT 138:231731

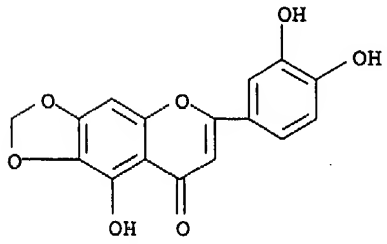
AB 3-Deoxyflavonoid compds. and methods for inhibiting T-cell activity and treating diseases and disorders (e.g., autoimmune disorders, inflammatory disorders, diabetes, ALS, MS, rheumatoid arthritis, etc.). In some cases the efficacy and/or duration of action of luteolin and/or other 3-deoxyflavonoid compds. may be increased by administering such compds. along with Rutin, a Rutin congener and/or a Rutin derivative Also, in some cases, first pass metabolism of luteolin or other 3-deoxyflavonoids may be avoided by administering such compds. by parenteral routes (e.g., sublingual, buccal, intranasal, injection, etc.).

IT **501445-13-2 501445-14-3 501445-15-4**
501445-16-5 501445-18-7 501445-19-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3-deoxyflavonoids that inhibit T-lymphocyte activation and use in treating immune disorders and inflammatory disorders)

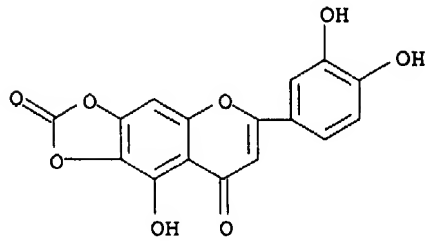
RN 501445-13-2 HCAPLUS
CN Acetic acid, 2,2'-[[4-[7-(carboxymethoxy)-5-hydroxy-4-oxo-4H-1-benzopyran-2-yl]-1,2-phenylene]bis(oxy)]bis- (9CI) (CA INDEX NAME)



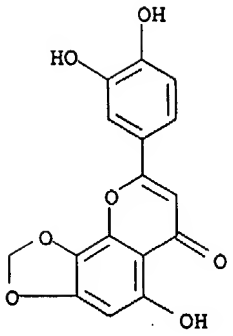
RN 501445-14-3 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 6-(3,4-dihydroxyphenyl)-9-hydroxy- (9CI) (CA INDEX NAME)



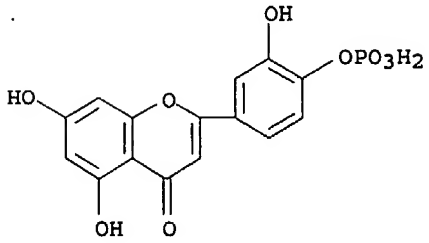
RN 501445-15-4 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-2,8-dione, 6-(3,4-dihydroxyphenyl)-9-hydroxy- (9CI) (CA INDEX NAME)



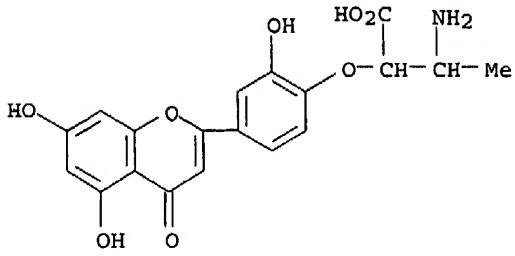
RN 501445-16-5 HCAPLUS
CN 6H-1,3-Dioxolo[4,5-h][1]benzopyran-6-one, 8-(3,4-dihydroxyphenyl)-5-hydroxy- (9CI) (CA INDEX NAME)



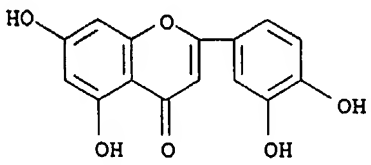
RN 501445-18-7 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-[3-hydroxy-4-(phosphonooxy)phenyl]-(9CI) (CA INDEX NAME)



RN 501445-19-8 HCAPLUS
CN Butanoic acid, 3-amino-2-[4-(5,7-dihydroxy-4-oxo-4H-1-benzopyran-2-yl)-2-hydroxyphenoxy]- (9CI) (CA INDEX NAME)



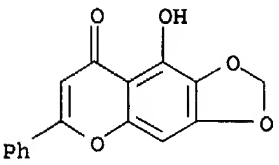
IT **491-70-3**, Luteolin
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3-deoxyflavonoids that inhibit T-lymphocyte activation and use in treating immune disorders, inflammatory disorders, and diabetes)
RN 491-70-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)



L29 ANSWER 8 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:652962 HCAPLUS
DOCUMENT NUMBER: 137:213533
TITLE: Microscopic studies on attachment and differentiation of zoospores of the phytopathogenic fungus Aphanomyces cochlioides
AUTHOR(S): Islam, Md. Tofazzal; Ito, Toshiaki; Tahara, Satoshi
CORPORATE SOURCE: Laboratory of Ecological Chemistry, Division of Applied Bioscience, Graduate School of Agriculture, Hokkaido University, Sapporo, 060-8589, Japan
SOURCE: Journal of General Plant Pathology (2002), 68(2), 111-117
CODEN: JGPPBQ; ISSN: 1345-2630
PUBLISHER: Phytopathological Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The mode of aggregation, attachment and differentiation of zoospores of the phytopathogenic fungus Aphanomyces cochlioides when interacting with the host and a host-specific attractant and a G-protein activator, mastoparan, was studied by light and SEM. When a zoospore approached very close to the host root, it seemed to halt, then coiled its anterior flagellum on its body. The halted zoospore appeared to contact the host surface with its posterior flagellum, which gradually drew the encysting zoospore onto the root surface. The spore then docked precisely on the root surface at its ventral face with the help of the posterior flagellum and anchored itself by releasing some adhesive materials. The adherent spore became a spherical after shedding its flagella and rapidly turned into an expanded cyst forming a smooth cyst coat around it, and finally changed into a smaller cystospore covered with a wrinkled surface. In contrast, the mastoparan- or cochliophilin A-stimulated zoospores on artificial membranes aggregated by using their posterior flagella before encystment. These contrasting phenomena suggest that A. cochlioides zoospores may use their posterior flagella for successful docking on the host surface or for aggregation of encysting spores in the absence of the host.
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 9 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:540648 HCAPLUS
DOCUMENT NUMBER: 137:275741
TITLE: Betalain and phenolic compositions of four beetroot (Beta vulgaris) cultivars
AUTHOR(S): Kujala, Tytti S.; Vienola, Maarit S.; Klika, Karel D.; Loponen, Jyrki M.; Pihlaja, Kalevi
CORPORATE SOURCE: Department of Chemistry, University of Turku, 20014, Finland
SOURCE: European Food Research and Technology (2002), 214(6), 505-510
CODEN: EFRTFO; ISSN: 1438-2377

PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Four cultivars of red beetroot (Beta vulgaris) were evaluated with respect to their betalain and phenolic contents. The compds. were analyzed using HPLC and identified by HPLC-DAD, HPLC-ESI-MS and NMR techniques. Betalains (vulgaxanthins I and II, betanin and isobetanin) and phenolics [5,5',6,6'-tetrahydroxy-3,3'-biindolyl, feruloylglucose and β-D-fructofuranosyl-α-D-(6-O-(E)-feruloylglucopyranoside)] were determined in different parts of the root; betalains were analyzed sep. in the water extract and phenolics in the fractionated 80% aqueous methanol extract (betalain-free water fraction). In each cultivar, both betanin and isobetanin were found in greater amts. in the peel than in the flesh. A similar trend was not observed in the distribution of vulgaxanthins. The three studied phenolics appeared in all root parts of the beetroot cultivars with the flesh generally containing the least content. Addnl., two phenolic amides (N-trans-feruloyltyramine and N-trans-feruloylhomovanillylamine) and four flavonoids (betagarin, betavulgarin, cochliophilin A and dihydroisorhamnetin) were detected in the fractionated 80% aqueous methanol peel exts. (acetonitrile fraction) of beetroot.
IT **110204-45-0**, Cochliophilin A
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(betalain and phenolic compns. of four beetroot cultivars)
RN 110204-45-0 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

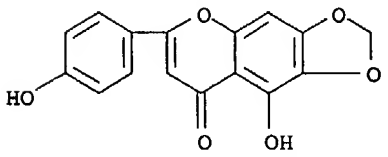
L29 ANSWER 10 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:523324 HCAPLUS
DOCUMENT NUMBER: 138:142301
TITLE: Isoflavonoids from the rhizomes of Belamcanda chinensis and their effects on aldose reductase and sorbitol accumulation in streptozotocin induced diabetic rat tissues
AUTHOR(S): Jung, Sang Hoon; Lee, Yeon Sil; Lee, Sanghyun; Lim, Soon Sung; Kim, Yeong Shik; Shin, Kuk Hyun
CORPORATE SOURCE: Natural Products Research Institute, Seoul National University, Seoul, 110-460, S. Korea
SOURCE: Archives of Pharmacal Research (2002), 25(3), 306-312
CODEN: APHRDQ; ISSN: 0253-6269
PUBLISHER: Pharmaceutical Society of Korea
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Aldose reductase, the key enzyme of the polyol pathway, is known to play important roles in the diabetic complication. The inhibitors of aldose reductase, therefore, would be potential agents for the prevention of diabetic complications. To evaluate active principles for the inhibition

of aldose reductase from the rhizomes of Belamcanda chinensis, 12 phenolic compds. were isolated and tested for their effects on rat lens aldose reductase. As a result, isoflavones such as tectorigenin, irigenin and their glucosides were found to show a strong aldose reductase inhibition. Tectoridin and tectorigenin, exhibited the highest aldose reductase inhibitory potency, their IC50 values, being 1.08 + 10-6 M and 1.12 + 10-6 M, resp., for DL-glyceraldehyde as a substrate. Both compds., when administered orally at 100 mg/kg for 10 consecutive days to streptozotocin-induced diabetic rats, caused a significant inhibition of sorbitol accumulation in the tissues such as lens, sciatic nerves, and red blood cells. Tectorigenin showed a stronger inhibitory activity than tectoridin. From these results, it is suggested that tectorigenin is attributed to be a promising compound for the prevention and/or treatment of diabetic complications.

IT **60948-17-6P**, Kanzakiflavone-2
RL: PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(isoflavonoids from rhizomes of Belamcanda chinensis on aldose reductase and sorbitol accumulation in diabetic rat tissues)

RN 60948-17-6 HCAPLUS

CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 11 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:670665 HCAPLUS

DOCUMENT NUMBER: 135:355322

TITLE: The third naturally occurring attractant toward zoospores of phytopathogenic Aphanomyces cochlioides from the Spinacia oleracea host plant

AUTHOR(S): Tahara, Satoshi; Ohkawa, Kaori; Takayama, Tomohiko; Ogawa, Yuko

CORPORATE SOURCE: Division of Applied Bioscience, Graduate School of Agriculture, Hokkaido University, Sapporo, 060-8589, Japan

SOURCE: Bioscience, Biotechnology, and Biochemistry (2001), 65(8), 1755-1760
CODEN: BBBIEJ; ISSN: 0916-8451

PUBLISHER: Japan Society for Bioscience, Biotechnology, and Agrochemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

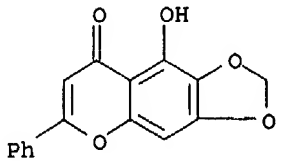
AB A bioassay-guided survey of spinach leaf constituents resulted in 5,4'-dihydroxy-3,3'-dimethoxy-6,7-methylenedioxyflavone (I) being identified as the third naturally-occurring attractant in the host plant toward the zoospores of its pathogen, Aphanomyces cochlioides. The isolate showed attracting activity around Chromosorb W AW particles (60-80

mesh) coated with a 10-5 M solution in a zoospore suspension. However, this activity was 1/100-1/1000 less than that of cochliophilin A, an attractant in the roots of spinach. Bioassays with the present isolate and related compds. revealed that 5,3',4'-trihydroxy-3-methoxy-6,7-methylenedioxyflavone did not possess attractant activity, but rather weak antagonistic activity toward the former two attractants from spinach.

IT **110204-45-0P**, Cochliophilin A
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(third naturally occurring attractant toward zoospores of phytopathogenic Aphanomyces cochlioides from Spinacia oleracea host plant)

RN 110204-45-0 HCAPLUS

CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 12 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:319108 HCAPLUS
DOCUMENT NUMBER: 135:1602
TITLE: Repellent activity of estrogenic compounds toward zoospores of the phytopathogenic fungus Aphanomyces cochlioides
AUTHOR(S): Islam, M. Tofazzal; Tahara, Satoshi
CORPORATE SOURCE: Division of Applied Bioscience, Graduate School of Agriculture, Hokkaido University, Sapporo, 060-8589, Japan
SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (2001), 56(3/4), 253-261
CODEN: ZNCBDA; ISSN: 0939-5075
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung
DOCUMENT TYPE: Journal
LANGUAGE: English

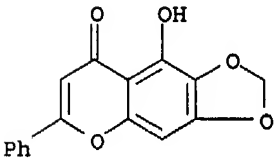
AB Bisphenol A, showed potent repellent activity against the zoospores of Aphanomyces cochlioides. Based on this finding, a number of androgenic and estrogenic compds. (e.g. testosterone, progesterone, estradiols, diethylstilbestrol, estrone, estriol, pregnenolone, dienestrol etc.) were tested on the motility behavior of A. cochlioides zoospores. Most of the estrogenic compds. exhibited potent repellent activity (1 μg/mL or less by the "particle method") toward the motile zoospores of A. cochlioides. The authors derivatized some of the estrogens and discussed the relationship between the structure of active mols. and their repellent activity. Aromatization of the A ring with a free hydroxyl group at C-3 position of a steroidal structure is necessary for higher repellent activity. Methylation of diethylstilbestrol (DES) yielded completely different activity i.e. both mono- and di-Me ethers of DES showed

attractant activity. The attracted zoospores were encysted and then germinated in the presence of di-Me ether of DES. The potential usefulness of this repellent test is discussed for the detection of estrogenic activity of naturally occurring compds., and the possible role of phytoestrogens in host/parasite interactions.

IT **110204-45-0**, Cochliophilin A
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(Aphanomyces cochlioides zoospore motility response to)

RN 110204-45-0 HCAPLUS

CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 13 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:103462 HCAPLUS

DOCUMENT NUMBER: 134:292704

TITLE: Simple flavones possessing complex biological activity

AUTHOR(S): Tahara, S.; Ingham, J. L.

CORPORATE SOURCE: Department of Applied Bioscience, Faculty of Agriculture, Hokkaido University, Sapporo, 060-8589, Japan

SOURCE: Studies in Natural Products Chemistry (2000), 22(Bioactive Natural Products (Part C)), 457-505
CODEN: SNPCE2

PUBLISHER: Elsevier Science B.V.

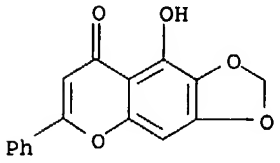
DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 87 refs. Two simple flavones, each of which exhibits distinct biol. activity despite their closely related structures, have been recognized by detailed bioassays, and bioassay-oriented isolation procedures. The identity of both flavones has been confirmed by synthesis. One of these compds., 5-methoxy-6,7-methylenedioxyflavone has been found in an extract of Polygonum lapathifolium L. subsp. nodosum (Polygonaceae) using a screening test devised to detect antidotes against the benzimidazole fungicide, benomyl (or its active principle MBC, 1H-benzimidazol-2-ylcarbamic acid Me ester). The other compound, 5-hydroxy-6,7-methylenedioxyflavone, is a host-specific signalling substance that exudes from spinach roots and attracts zoospores of the phytopathogenic fungus Aphanomyces cochlioides the cause of spinach root rot. This review describes the bioassay, isolation and identification of these active compds., and compares their activity with that of various other related, and unrelated, chems. of either plant or synthetic origin. The possible ecochem. role and mode of action of flavone and non-flavone antidotes and attractants is briefly discussed.

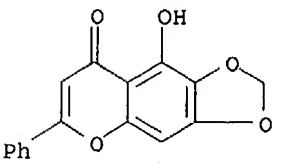
IT **110204-45-0**, 5-Hydroxy-6,7-methylenedioxyflavone
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)
(plant flavones possessing complex biol. activity)
RN 110204-45-0 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

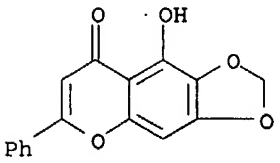
L29 ANSWER 14 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:192630 HCAPLUS
DOCUMENT NUMBER: 130:264755
TITLE: Plant secondary metabolites regulating behavior of zoospores of the phytopathogenic fungus Aphanomyces cochlioides
AUTHOR(S): Tahara, Satoshi; Mizutani, Masanori; Takayama, Tomohiko; Ohkawa, Kaori
CORPORATE SOURCE: Dep. of Applied Bioscience, Faculty of Agriculture, Hokkaido University, Sapporo, 060-8589, Japan
SOURCE: Pesticide Science (1999), 55(2), 209-211
CODEN: PSSCBG; ISSN: 0031-613X
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A number of compds. isolated from various plant species were tested for their ability to affect the mobility of zoospores of A. cochlioides which causes root rot in spinach (Spinacia oleracea). Compds. may act as attractants, repellents or stimulants of zoospore movement or they may halt movement by causing the spore to clump and settle. Bioassays revealed compds. with these modes of action, as well as some which acted directly on the fungus.
IT **110204-45-0P**, Cochliophilin a
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(plant secondary metabolite with activity on Aphanomyces cochlioides zoospores)
RN 110204-45-0 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 15 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:587939 HCAPLUS
DOCUMENT NUMBER: 129:327812
TITLE: Drop method as a quantitative bioassay method of chemotaxis of Aphanomyces cochlioides zoospore
AUTHOR(S): Takayama, Tomohiko; Mizutani, Junya; Tahara, Satoshi
CORPORATE SOURCE: Dep. Applied Bioscience, Fac. Agriculture, Hokkaido Univ., Sapporo, 060-8589, Japan
SOURCE: Nippon Shokubutsu Byori Gakkaiho (1998), 64(3), 175-178
CODEN: NSBGAM; ISSN: 0031-9473
PUBLISHER: Nippon Shokubutsu Byori Gakkai
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A drop method using fluorinated hydrocarbon (FC-72) was successfully applied as a quant. assay to determine the threshold concentration of cochliophilin A, a potent Aphanomyces cochlioides zoospore attractant originally isolated from spinach roots. This method revealed that the number of zoospores attracted to droplets containing cochliophilin A increased with time, until approx. 60 to 90 s after injection of the droplet into a zoospore suspension. The threshold concentration, above which cochliophilin A was able to function as a zoospore attractant, was determined to be .apprx.3.0+10-9 M. Interestingly, zoospores attracted to droplets containing cochliophilin A at a concentration greater than 1.1+10-7 M massed on the surface of the droplets, a behavior that was quite similar to that observed on the root surface of host plants. This result suggested that the drop method would be useful not only as a quant. assay of chemotaxis, but also as a technique to investigate the mechanism of zoospore massing.
IT **110204-45-0**, 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl-
RL: ANT (Analyte); ANST (Analytical study)
(drop method as a quant. bioassay method of chemotaxis of Aphanomyces cochlioides zoospore)
RN 110204-45-0 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

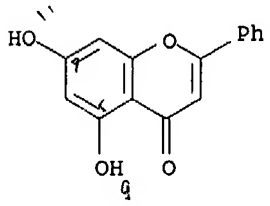
L29 ANSWER 16 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:978211 HCAPLUS
DOCUMENT NUMBER: 124:23827
TITLE: Activity of host-derived attractants and their related compounds toward the zoospores of phytopathogenic Aphanomyces cochlioides

AUTHOR(S): Kikuchi, Hiroto; Horio, Takeshi; Kawabata, Jun; Koyama, Noriyuki; Fukushi, Yukiharu; Mizutani, Junya; Tahara, Satoshi
CORPORATE SOURCE: Department of Applied Bioscience, Hokkaido University, Sapporo, 060, Japan
SOURCE: Bioscience, Biotechnology, and Biochemistry (1995), 59(11), 2033-5
CODEN: BBBIEJ; ISSN: 0916-8451
PUBLISHER: Japan Society for Bioscience, Biotechnology, and Agrochemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

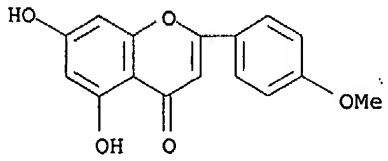
AB Eleven flavones, including cochliophilin A and a chromone, were chemical prepared to determine the attracting activity for zoospores of Aphanomyces cochlioides, a causative fungus of spinach root rot. Analyses of the structure-activity relationship of each revealed a significant correlation between the zoospore attracting activity and the A-ring oxygenation at C-5 and C-7 in flavone skeleton. The relative attractancy of 4 regioisomers of N-trans-feruloyl 4-O-methyldopamine, which was identified as a zoospore attractant specific to another host plant Chenopodium album, was also examined

IT **480-40-0**, 5,7-Dihydroxyflavone **480-44-4**, 5,7-Dihydroxy-4'-methoxyflavone **491-67-8**, 5,6,7-Trihydroxyflavone **491-78-1**, 5-Hydroxyflavone **520-28-5**, 5-Hydroxy-7-methoxyflavone **740-33-0**, 5-Hydroxy-6,7-dimethoxyflavone **5128-44-9**, 5-Hydroxy-7,4'-dimethoxyflavone **93322-08-8 110204-45-0**, Cochliophilin A
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(activity of host-derived attractants and their related compds. toward the zoospores of phytopathogenic Aphanomyces cochlioides)

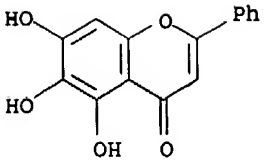
RN 480-40-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 480-44-4 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

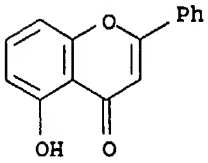


RN 491-67-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl- (9CI) (CA INDEX NAME)

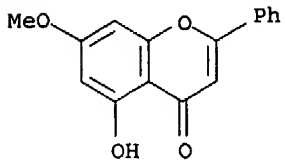


Excluded

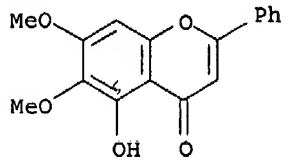
RN 491-78-1 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



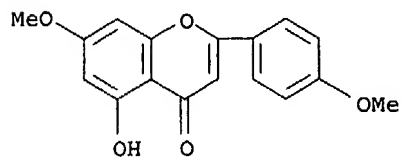
RN 520-28-5 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-7-methoxy-2-phenyl- (9CI) (CA INDEX NAME)



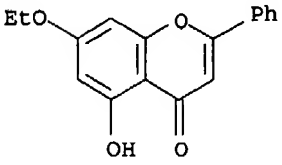
RN 740-33-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-6,7-dimethoxy-2-phenyl- (9CI) (CA INDEX NAME)



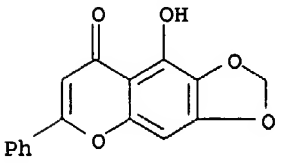
RN 5128-44-9 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-7-methoxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



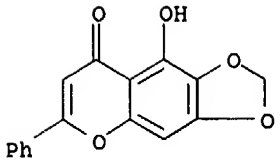
RN 93322-08-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 7-ethoxy-5-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 110204-45-0 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



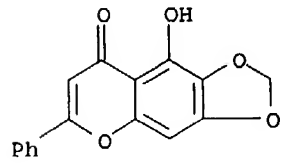
L29 ANSWER 17 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:25511 HCAPLUS
DOCUMENT NUMBER: 120:25511
TITLE: Naturally occurring antidotes against benzimidazole fungicides
AUTHOR(S): Tahara, Satoshi; Matsukura, Yumiko; Katsuta, Hiroyuki; Mizutani, Junya
CORPORATE SOURCE: Fac. Agric., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1993), 48(9-10), 757-65
CODEN: ZNCBDA; ISSN: 0341-0382
DOCUMENT TYPE: Journal
LANGUAGE: English
AB TLC bioautog. using precoated glass thin-layer plates impregnated with benomyl or carbendazim (MBC), and Cladosporium herbarum as a test fungus, was evaluated as a facile way to detect plant secondary metabolites antidoting against benzimidazole fungicides. In addition to emodin and α-tocopherol from Polygonum sachalinense, three phenolics, 3,5-dihydroxy-4-methylstilbene and 5-methoxy-6,7-methylenedioxyflavone from P. lapathifolium and 2,6-dimethoxybenzoquinone from P. thunbergii, were isolated and characterized as new benzimidazole antidotes. Emodin exhibited the antidoting activity not only against benomyl but also against MBC, thiabendazole, thiophanate-Me and nocodazole. Furthermore, emodin showed antidoting activity against MBC in the wild-type Neurospora crassa and against diethofencarb in the mutant of N. crassa resistant to benzimidazole fungicides but highly susceptible to diethofencarb.
IT **110204-45-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)
RN 110204-45-0 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



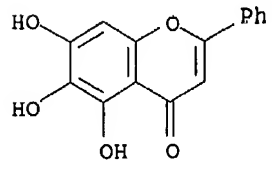
L29 ANSWER 18 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:466159 HCAPLUS
DOCUMENT NUMBER: 117:66159
TITLE: A potent attractant of zoospores of Aphanomyces cochlioides isolated from its host, Spinacia oleracea
AUTHOR(S): Horio, T.; Kawabata, Y.; Takayama, T.; Tahara, S.; Kawabata, J.; Fukushi, Y.; Nishimura, H.; Mizutani, J.
CORPORATE SOURCE: Fac. Agric., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Experientia (1992), 48(4), 410-14
CODEN: EXPEAM; ISSN: 0014-4754
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A highly potent attractant of zoospores of A. cochlioides, a causal fungus of the root rot disease of spinach (S. oleracea), was isolated from spinach roots, and its structure was determined by spectroscopic evidence and chemical synthesis as cochliophilin A (5-hydroxy-6,7-methylenedioxyflavone, I). A chromosorb particle prepared by soaking in I solution showed a potent attracting activity toward the zoospores using concns. of I above 10-9 or 10-10 M.

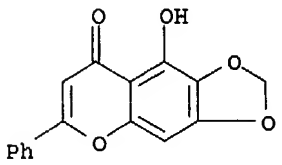
IT **110204-45-0**, Cochliophilin A
RL: BIOL (Biological study)
(as chemoattractant for zoospores of Aphanomyces cochlioides, structure of)
RN 110204-45-0 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



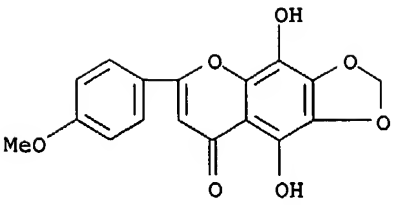
IT **491-67-8**
RL: BIOL (Biological study)
(in cochliophilin A preparation)
RN 491-67-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



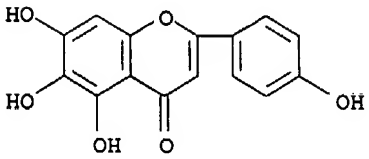
L29 ANSWER 19 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:531082 HCAPLUS
DOCUMENT NUMBER: 107:131082
TITLE: New flavonoids isolated from infected sugarbeet roots
AUTHOR(S): Takahashi, Hajime; Sasaki, Teruji; Ito, Masaaki
CORPORATE SOURCE: Dep. Gen. Educ., Higashi Nippon Gakuen Univ., Tobetsu, 061-02, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1987), 60(6), 2261-2
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB New flavonoid compds. 3,5-dihydroxy-6,7-methylenedioxyflavanone, 2',5-dihydroxy-6,7-methylenedioxyisoflavone, and 5-hydroxy-6,7-methylenedioxyflavone were isolated from sugar beet roots infected with Rhizoctonia solani.
IT **110204-45-0**
RL: BIOL (Biological study)
(from Rhizoctonia solani infected sugar beet roots)
RN 110204-45-0 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-phenyl- (9CI) (CA INDEX NAME)



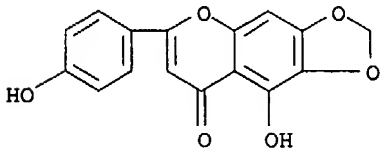
L29 ANSWER 20 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:406890 HCAPLUS
DOCUMENT NUMBER: 101:6890
TITLE: Synthetic studies of the flavone derivatives. VIII. Synthesis of kanzakiflavones and their isomers
AUTHOR(S): Iinuma, Munekazu; Tanaka, Toshiyuki; Matsuura, Shin
CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, 502, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1984), 32(3), 1006-10
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Kanzakiflavone-1 and -2, (I, R = H, R1R2 = OCH2O, R3 = OH, R4 = Me; R = R3 = R4 = H, R1R2 = OCH2O) isolated from Iris unguicularis, and their positional isomers I (R = R1 = R4 = H, R2 = R3 = OH, R2R3 = OCH2O; R = R4 = H, R1 = R2 = OH, R3 = H, OH; R = R4 = Me, R1R2 = OCH2O, R3 = OMe; R = R4 = Me, R1 = OMe, R2R3 = OCH2O) were synthesized to confirm the structures of the isolates. The differences among these flavones are discussed on the basis of spectral data.
IT **59870-76-7**
RL: PRP (Properties)
(mol. structure of)
RN 59870-76-7 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 4,9-dihydroxy-6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT **529-53-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylenation of)
RN 529-53-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



IT **60948-17-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, methylation, and mol. structure of)
RN 60948-17-6 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



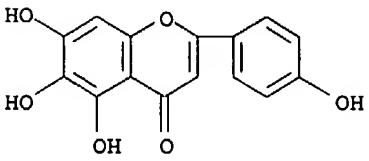
L29 ANSWER 21 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:597277 HCAPLUS
DOCUMENT NUMBER: 89:197277
TITLE: Synthesis of kanzakiflavones
AUTHOR(S): Bhardwaj, D. K.; Jain, S. C.; Sharma, G. C.; Singh, R.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1978), 16B(4), 339-40
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The structures of kanzakiflavone 1 and 2 were confirmed as 5,8-dihydroxy-4'-methoxy-6,7-methylenedioxyflavone (I) and 5,4'-dihydroxy-6,7-methylenedioxyflavone (II), resp., by their syntheses. Methylenation of 5,6,7-trihydroxy-4'-methoxyflavone obtained from 4'-benzyloxy-2,5-dihydroxyacetophenone, followed by hydroxylation of the resulting 5-hydroxy-4'-methoxy-6,7-methylenedioxyflavone gave I. Methylenation of scutellarein gave II.

IT **529-53-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylenation of)

RN 529-53-3 HCAPLUS

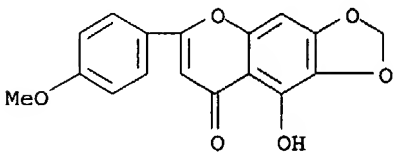
CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



IT **63934-55-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydroxylation of)

RN 63934-55-4 HCAPLUS

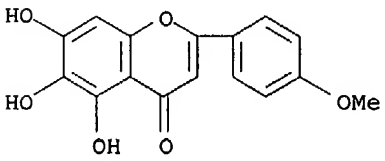
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT **6563-66-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylenation of)

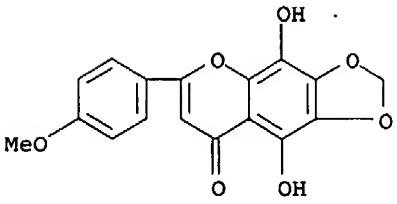
RN 6563-66-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

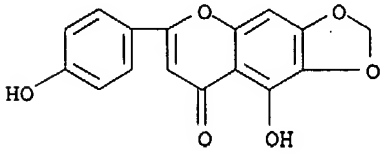


IT **59870-76-7P 60948-17-6P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

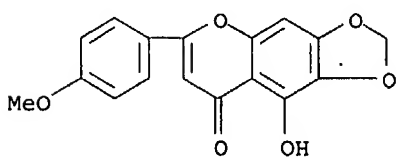
(synthesis of)
RN 59870-76-7 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 4,9-dihydroxy-6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



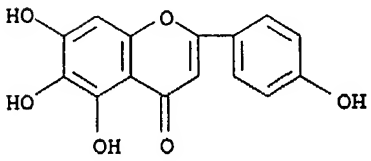
RN 60948-17-6 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



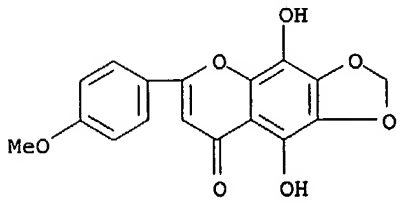
L29 ANSWER 22 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:502123 HCAPLUS
DOCUMENT NUMBER: 87:102123
TITLE: Synthesis of kanzakiflavone-1 and kanzakiflavone-2
AUTHOR(S): Manchanda, V. P.; Khanna, R. N.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, India
SOURCE: Current Science (1977), 46(13), 445-6
CODEN: CUSCAM; ISSN: 0011-3891
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Kanzakiflavone-1 (I; R1 = R2 = H) was prepared by treatment of scutellarein with CH2I2, Me2CO and K2CO3. Treatment of I (R1 = R2 = H) with Me2SO4, Me2CO and K2CO3 gave I (R1 = H, R2 = Me), which was treated with aqueous KOH, pyridine, and K2S2O8 to give kanzakiflavone-2 (I; R1 = OH, R2 = Me).
IT **63934-55-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to kanzakiflavone-1)
RN 63934-55-4 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



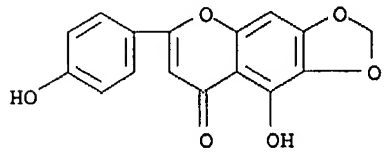
IT **529-53-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylene iodide)
RN 529-53-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



IT **59870-76-7P 60948-17-6P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of)
RN 59870-76-7 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 4,9-dihydroxy-6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

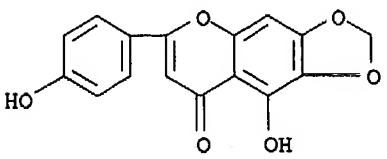


RN 60948-17-6 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

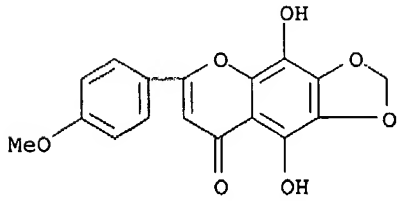


L29 ANSWER 23 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:592495 HCAPLUS
DOCUMENT NUMBER: 85:192495
TITLE: Studies on constituents of genus Iris. VIII. The constituents of Iris unguicularis Poir. (2)
AUTHOR(S): Arisawa, Munehisa; Kizu, Haruhisa; Morita, Naokata
CORPORATE SOURCE: Fac. Pharm. Sci., Toyama Univ., Toyama, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1976), 24(7), 1609-12
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal

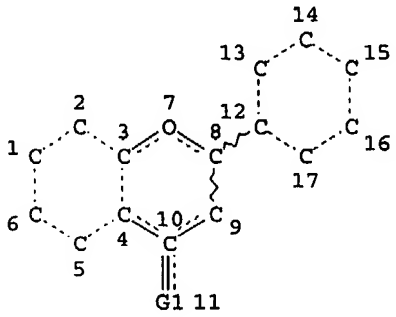
LANGUAGE: English
AB Kanzakiflavone-2 (I), a new flavone, was isolated from the ethereal extract and 3 known compds., iridin, mangiferin, and isomangiferin were isolated from the butanolic extract of I. unguicularis. The structure of I was determined
by chemical and spectral means.
IT **60948-17-6P**
RL: PREP (Preparation)
(from Iris unguicularis)
RN 60948-17-6 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 9-hydroxy-6-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L29 ANSWER 24 OF 24 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:417131 HCAPLUS
DOCUMENT NUMBER: 85:17131
TITLE: Studies on constituents of genus Iris. VII. The constituents of Iris unguicularis Poir.
AUTHOR(S): Arisawa, Munehisa; Morita, Naokata
CORPORATE SOURCE: Fac. Pharm. Sci., Toyama Univ., Toyama, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1976), 24(4), 815-17
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Kanzakiflavone-1(I), C17H12O7, mp 291-3°, a new flavone, has been isolated from the rhizomes of I. unguicularis (Japanese name: Kanzakiayame) together with irigenin and iristectorigenin A. The structure of I has been determined as 5,8-dihydroxy-4'-methoxy-6,7-methylenedioxyflavone by chemical and spectral means.
IT **59870-76-7**
RL: BIOL (Biological study)
(a new flavone)
RN 59870-76-7 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 4,9-dihydroxy-6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



=> d que l24
L1 STR



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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
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L22 STR

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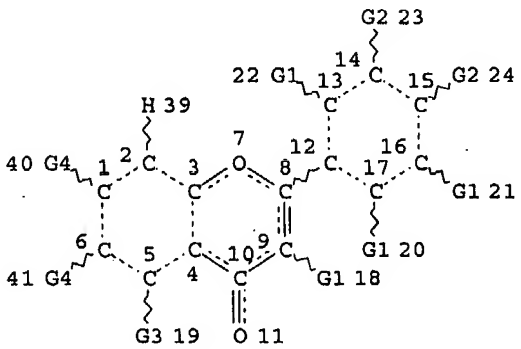
S~Me @37 38



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N @82

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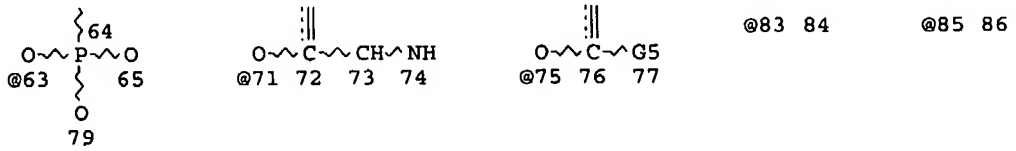
Ak~N Cb~N

Page 1-A



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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 79

STEREO ATTRIBUTES: NONE
L23 1475 SEA FILE=REGISTRY SUB=L2 SSS FUL L22
L24 10057 SEA FILE=HCAPLUS ABB=ON PLU=ON L23

=> d l24 ibib ab hitstr 10040-10057 ← only a small sample of old references printed.

L24 ANSWER 10040 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1925:18058 HCAPLUS

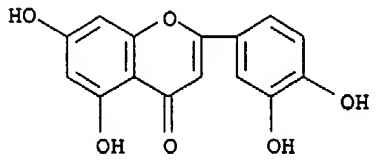
DOCUMENT NUMBER: 19:18058
ORIGINAL REFERENCE NO.: 19:2341c-i
TITLE: Synthesis of pyrylium salts of anthocyanidin type. VI. Polyhydroxyflavylium salts related to chrysin, apigenin, lotoflavin, luteolin, galangin, flsetin and morin
AUTHOR(S): Pratt, D. D.; Robinson, Robert
SOURCE: Journal of the Chemical Society, Abstracts (1925), 127, 1128-38
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C. A. 19, 1141. Ph 2-hydroxy-4,6-dimethoxystyryl ketone, pale yellow, m. 136°, in 5 g. yield from 6 g. 2,4,6-HO(MeO)2CeH2CHO and 4 g. BzMe in MeOH-KOH; heating with concentrated HCl gives dimethylchrysinidin chloride; the iodide forms red microneedles. The chloride, heated with HI in PhOH, gives chrysinidin iodide, bright red needles, converted by AgCl into the chloride, orange-yellow, with 2H2O, darkens 130°, does not m. 300°. The yellow concentrated H2SO4 solution exhibits a week green fluorescence. The color base is red; its aqueous Na2CO3 solution is red but the color is neither intense nor persistent on dilution Perchlorate, orange-yellow, darkens 178°, m. 185° (decomposition). 5,7,4'-Trimethoxyflavylium chloride with HI in PhOH gives the iodide, which is converted by AgCl into apigeninidin chloride, red needles with 2H2O, darkens 180°, does not m. 300°. A film on glass has a fine green luster. The orange-red EtOH solution has a weak green fluorescence, while the yellow H2SO4 solution has a bright fluorescence. The color base has a port wine-red color, soluble in Na2CO3 or NH4OH to a rich damson solution In NaOH the ring is easily broken and acids precipitate a chalcone, converted by mineral acids to the pyrylium salt. Perchlorate, orange-yellow, darkens 190°, softens 220°, decomps. 222°. 2,4-Dimethoxyphenyl 2-hydroxy-4,6-dimethoxystyryl ketone, pale yellow, m. 154°, forms a red K salt and with concentrated HCl gives 5,7,2',4'-tetramethoxyflavylium chloride, red needles, decomps. 134°; ferrichloride, red needles, decomps. 180°; the yellow H2SO4 solution exhibits a green fluorescence, also characteristic of the orange-pink iso-AmOH solution HI in PhOH, as above, gives lotoflavinidin chloride, orange-yellow needles with 2 H2O, darkens 190°, does not m. 300°; the color base is deep red and the alkaline solution reddish violet. 5,7,3',4'-Tetramethoxyflavylium chloride gives rise to luteolinidin chloride, reddish brown, with 2 H2O, darkens 200°, does not m. 300°; the red EtOH solns. are devoid of fluorescence; the yellow H2SO4 solution has a faint green fluorescence; the aqueous solns. are colored magenta, bluish violet and pure blue by AcONa, Na2CO3, and NaOH, resp. The FeCl3 reaction is violet-blue in EtOH, reddish violet in H2O. 3,5,7-Trimethoxyflavylium chloride and HI give a golden brown iodide, C15H11O4I.HI.3H2O, m. 145°, changed by AgCl to galanginidin chloride. 7-Hydroxy-3,3',4'-trimethoxyflavylium chloride gives fisetinidin chloride, reddish brown, with 0.5 H2O, which resembles cyanidin in its color reactions. It, however, does not melt when plunged into a bath at 222°; solns. of the violet color base have a redder tinge than those of cyanidin; the blue FeCl3 color fades more rapidly; the blue alkaline solns. are more unstable; the yellow-orange H2SO4 solns. have an apple-green fluorescence which becomes dark green on standing. 3,5,7,2',4'-Pentamethoxyflavylium chloride, red needles with green reflex, decompose 155°; ferrichloride, bright red needles, decompose

194°. HI gives morinidin chloride. The blue alkaline solns. of many anthocyanidins are dichroic and even if blue in thin layers or when dilute the color is bluish violet to reddish violet to red in thicker layers or in greater concentration This dichroism is especially characteristic of alkaline solns. of morinidin.

IT **491-70-3**, Luteolin **520-36-5**, Apigenin
(polyhydroxyflavylium salts related to)

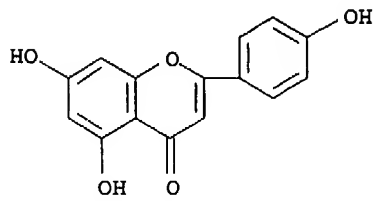
RN 491-70-3 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)



RN 520-36-5 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L24 ANSWER 10041 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1924:7255 HCAPLUS

DOCUMENT NUMBER: 18:7255

ORIGINAL REFERENCE NO.: 18:986a-e

TITLE: Synthesis of pyrylium salts of anthocyanidin type. IV. Flavylium salts related to chrysin, apigenin and luteolin

AUTHOR(S): Pratt, D. D.; Robinson, R.; Williams, P. N.

SOURCE: Journal of the Chemical Society, Abstracts (1924), 125, 199-207
CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

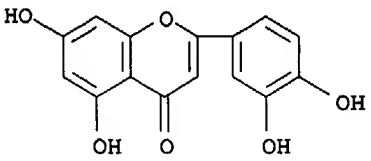
AB Dimethylchrysinidin ferrichloride, reddish brown, m. 178°, results from 2,4,6-HO(MeO)2C6H2CHO and BzMe. The bright yellow H2SO4 solution exhibits a green fluorescence, becoming more intense on standing. AcONa ppts. a colorless pseudo-base. p-Anisyl β-hydroxyvinyl ketone (I), from p-AcC6H4OMe and HCO2Et, very unstable and undergoes autocondensation when in Et2O solution It was analyzed as the Cu salt, green prisms, m. 206-7°. The Et2O solution of the above ketone and m-C6H4(OH)2, condensed by HCl, yield 7-hydroxy-4'-methoxy-2-phenylbenzopyrylium chloride, brownish red, m. 182-3°, also obtained from

β-resorcylaldehyde and p-AcC6H4OMe. The yellow solution in H2SO4 or AcOH exhibits a brilliant green fluorescence. The FeCl3 salt was amorphous but the picrate, golden yellowish brown, m. 219-21° (decomposition), is crystalline Acacetidin chloride, from I and 1,3,5-C6H3(OH)3, brown prisms with green glance, does not m. 360°. The color base, best obtained by the action of AcONa, is purplish black, soluble in AcOEt with a reddish brown and in aqueous Na2CO3 with an intense bordeaux-red color. The sulfate is orange-red, the iodide, deep red, the perchlorate, orange-red, the mercuri-chloride, pale orange. Trimethylapigenidin ferrichloride, reddish brown with a green reflex, sinters 180°, m. 187°. The yellow H2SO4 solution develops a green fluorescence on standing. 2-Hydroxy-4,6-dimethoxystyryl 3,4-dimethoxyphenyl ketone, bright yellow, m. 178-9° with decomposition to a red oil, results by condensing 2,4,6-HO(MeO)2C6H2CHO and acetoveratrone with alc. KOH. The orange-red H2SO4 solution, on dilution with H2O, gradually deposits tetramethylluteolidin sulfate, orange-red; HBr gives the red bromide, having a green reflex. The chloride forms glistening red needles, which give the ferrichloride, salmon-red needles, m. 206-7°.

IT **491-70-3**, Luteolin **520-36-5**, Apigenin
(flavylium salts related to)

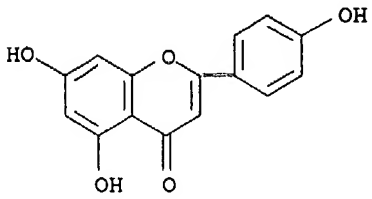
RN 491-70-3 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)



RN 520-36-5 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L24 ANSWER 10042 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	1923:23037 HCAPLUS
DOCUMENT NUMBER:	17:23037
ORIGINAL REFERENCE NO.:	17:3506c-i,3507a
TITLE:	Baicalin, a new flavone-glucuronic acid compound from the roots of Scutellaria baicalensis
AUTHOR(S):	Shibata, Keita; Iwata, Shojiro; Nakamura, Maxoto
SOURCE:	Acta Phytochimica (1923), 1, 105-39
	CODEN: APCJA8; ISSN: 0365-5393

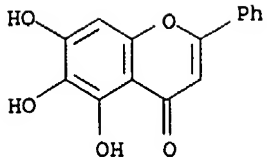
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The name scutellarin was applied by Takahashi to a crystalline compound from Scutellaria baicalensis, to which he ascribed the formula C10H8O3 (Arb. pharmakal. Inst. 239-43; Chemical Zentr. 1889, II, 100). The same name has, however, been accepted for a flavone-glueuronic acid compound found by Molisch and Goldschmiedt (Monatsh. 22, 679-99(1901)) in other species of Scutellaria, and it is proposed to call T.'s compound wogonin (from "wogon," the Japanese term for the root). A new compound, baicalin, closely allied to scutellarin, occurs in the roots of S. baicalensis, and can be extracted from the roots by boiling 50% alc., the yield being 12.5% of the weight of dry root. It is bright yellow, C21H18O11, m. 223°. When hydrolyzed with concentrated H2SO4, it is decomposed into glucuronic acid and a flavone derivative, baicalein, C15H10O5, yellow, m. 264-5° (decomposition). A great deal of evidence indicates that baicalein is a trihydroxyflavone, a hydroxychrysin with all 3 hydroxy groups in the one phenyl ring. By alkaline hydrolysis, baicalin gives PhCOMe, and when fused with KOH both baicalin and baicalein give BzOH. Baicalein appears to be identical with the 5,6,7-trihydroxy- flavone, prepared synthetically by Bargellini, C. A. 14,1527. Evidence that condensation with glucuronic acid to form baicalin takes place at the 6-HO group is furnished by the observation that baicalin is not oxidized by chloropentamminecobaltichloride, which gives a strong color reaction with o-di-HO compds. but not with corresponding m-compds. Scutellarin likewise fails to give a reaction with this reagent, and must therefore be constituted similarly to baicalin. Pentabenzoylscutellarin, m. 237-8° (decomposition). Baicalin gives with FeCl3 in alc. a dark green color, and with Pb(OAC)2, an orange-red precipitate It dissolves in alkalies with a yellow color, and reduces NH3-AgNO3 in the cold. It is difficult to alkylate, but forms with CH2N2 in acetone a mono-Me derivative, m. 211-12° (decomposition); this contains a free CO2H group. Dibromobaicalin softens above 270°. Baicalin is l-rotatory, [α]D18 -144.9°. Tetracetylbaicalin, prisms containing H2O, m. 256-7°. The fact that only a tetra-Ac derivative is formed indicates that the glucuronic acid is in the lactone form. A small quantity of what appeared to be a pentaacettylbaicalin, m. 212-13° (decomposition), was also obtained. Tetrabenzoylbaicalin, gray, m. 220-30°. Tribenzoylbaicalein, m. 199.5°. Triacetylbaicalein agrees in properties with Bargellini's tri-Ac derivative of 5,6,7-trihydroxyflavone (loc. cit.). Free baicalein is present with baicalin in the roots of the plant. Further investigation of wogonin shows that the substance as analyzed by T. contained water of crystallization The correct formula is C16H12O4, and it contains a MeO group. Acetylwogonin, C18H14O6, m. 152-3°; benzoylwogonin, yellowish white, m. 170°; methylwogonin, C16H11O3.OMe.H2O, yellowish white, m. 180-1°. Baicolein and scutellarein, like other hydroxyflavones (cf. C. A. 17, 3451) show two absorption bands in the ultra-violet, the bands showing shifts such as would be expected from the constitutions of the compds. In baicalin, the first band disappears, only a broad band at 3500 remaining, but in scutellarin both bands persist, perhaps through the influence of the 4'-HO group. Wogonin has an unusual spectrum with only one band, at 3500, but acetylwogonin, like triacetylbaicalein, shows the true flavone spectrum. The green parts of S. baicalensis contain scutellarin. The relation between the scutellarin of the leaves and the baicalin of the roots is a question of great biochem. interest.

IT **491-67-8**, Baicalein **21967-41-9**, Baicalin
(preparation of)

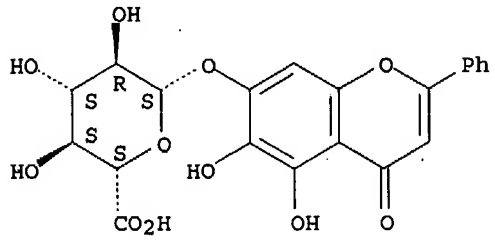
RN 491-67-8 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 21967-41-9 HCAPLUS
CN β-D-Glucopyranosiduronic acid, 5,6-dihydroxy-4-oxo-2-phenyl-4H-1-benzopyran-7-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 10043 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1923:22741 HCAPLUS
DOCUMENT NUMBER: 17:22741
ORIGINAL REFERENCE NO.: 17:3451i,3452a-c
TITLE: The absorption spectra of vegetable dyes of the flavone series. I
AUTHOR(S): Shibata, Yuji; Kimotsuki, Kensho
SOURCE: Acta Phytochimica (1923), 1, 91-104
CODEN: APCJA8; ISSN: 0365-5393
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

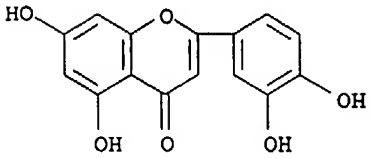
AB The vegetable coloring matters of the flavone series show two characteristic absorption curves in the ultraviolet, and since the position of these bands is affected by the number and orientation of the hydroxyl groups, the ultra-violet absorption spectra serve as a ready means of identifying the different members of the series. The observations are best made in 0.0001 M alc. solution Flavone itself has the two bands at frequencies 3500 and 4050. The position of the second band is scarcely influenced by hydroxyl groups, but the first is shifted towards the red by hydroxyl groups in the benzopyrone nucleus, and in the opposite direction by hydroxyl in the side phenyl group. Moreover, the depth of this band increases with the number of hydroxyl groups, as in the series kaempferol, quercetin, myricetin, containing, resp., one, two, and 3 hydroxyls in the side Ph group. Acetylation neutralizes the influence of the hydroxyl groups, and diacetylehrysin and pentaacetylquercetin have exactly the same absorption spectrum as flavone. In chrysin, apigenin, and luteolin, the head of the first absorption band is near 3500; chrysin is exceptional in that the second band is also shifted considerably towards the red. Galangin, kaempferol, and kaemp-feride form a closely related group with the first band at 2650. In quercetin, isorhamnetin, and myricetin, this band is also at 2650 but is deeper. The absorption

bands of the flavone coloring matters from 17 different plants were examined, and by comparison of the curves obtained with those of the above substances it was possible to determine to what type the unknown substances belonged. Exact correspondence was not obtained, probably on account of impurities in the plant prepns.

IT **491-70-3**, Luteolin **520-36-5**, Apigenin
(spectrum of)

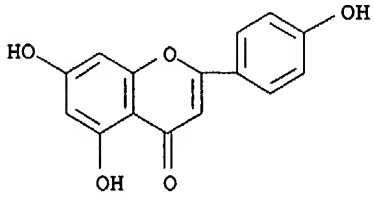
RN 491-70-3 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)



RN 520-36-5 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L24 ANSWER 10044 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1920:8270 HCAPLUS

DOCUMENT NUMBER: 14:8270

ORIGINAL REFERENCE NO.: 14:1527a-i,1528a-f

TITLE: 1,2,3-Trihydroxyflavone. Contribution to the knowledge of the constitution of scutellarein

AUTHOR(S): Bargellini, G.

CORPORATE SOURCE: Univ. Rome

SOURCE: Gazzetta Chimica Italiana (1919), 49, II, 47-63
CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal

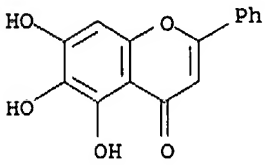
LANGUAGE: Unavailable

AB In a previous paper on the synthesis of scutellarein (A) (C. A. 9, 2237) B. confirmed the hypothesis of Goldschmiedt (Monatsh. 22, 679 (1901)), that A is a derivative of 1,2,3,5-C6H2(OH)4 (tetrahydroxyflavone) but could not determine which of the 2 possible formulas was correct. Considering the difficulty of solving this problem by direct expts. on A, B. has sought for indirect ways of determining which formula is to be selected. In this connection B. reviews work of Nierenstein (C. A. 6, 751, 1297, 7, 1715; II, 1134) on the oxidation of natural yellow hydroxyketonic coloring matters (xanthones, flavones, flavonols) into derivs. of phloroglucinol and 1,2,3,5-C6H2(OH)4. He points out that his own earlier expts. on the oxidation of apigenin (trihydroxyflavone) with CrO3 in AcOH by which he

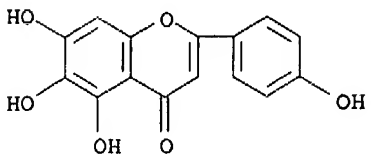
obtained hydroxyapigenin, which he thought was a derivative of 1,2,3,5-C6H2(OH)4, have not been completed owing to interruption due to the war. B. reports another series of expts. however, which contribute to this problem of the constitution of A. Starting with 2,3,4,6-(MeO)4C6HCOMe, he obtained the corresponding trihydroxyflavone (B) by condensing first with BzOMe in presence of Na and then saponifying the 2,3,4,6-tetramethoxybenzoylacetophenone (I), obtained with HI. This reaction is similar to that previously used for the synthesis of A and may give rise to 1 of 2 isomeric forms for B, II or III. Although in the case of A it is still impossible to determine which of the corresponding isomeric formulas is the correct one this is not true with B since one of the formulas, II, is that of the hydroxycrisine (C) of Nierenstein. C m. 304-5° while B m. about 265°. The Ac derivative of C m. 214-7°, while that of B m. 190-2°. Accordingly if C is really II then by exclusion B is III. Thus when I is saponified with HI the tetra-HO derivative reacts in such a way that H2O is eliminated between the OH at 6 and the enolic OH. The OH at 2 which could presumably react, similarly to give the other isomer does not do so. This may be explained on the basis of steric hindrance. The OMe at 2 lies between the 3-carbon chain at 1 and the OMe at 3 and is saponified more slowly than the OMe at 6, which adjoins the empty position at 5. When I is treated with HI the OH at 6 is freed first and reacts with the enolic OH before the OH at 2 is available. This was proved exptly. by showing that partial saponification gives the 1,2,3-trimethoxyflavone (IV). IV by further treatment with HI gives III. Using the same argument and assuming the analogy to hold the formula for A would be V. 2,3,4,6-(MeO)4C6HCOMe (D) was prepared by the method previously described (C. A. 5, 3806) by treating 1,2,3,5-C6H2(OMe)4 in CS2 with AcCl and AlCl3. Owing to the saponifying action of AlCl3 a tri-Me ether and a di-Me ether of 2,3,4,6-(HO)4C6HCOMe are formed as secondary products. Later (C. A. 99, 2238), B. obtained tri-Me and tetra-Me ethers of the corresponding propiophenone and benzophenone derivs. Nierenstein (C. A. 11, 1134) obtained D but instead of m. 43-5° he found its m. p. at 92-3°. B.'s product b. 310° and m. 43-5° and in no case could he obtain a product with the m. p. 92-3°. B. suggests that possibly N.'s compound is a compound methylated on the C. The semicarbazone of D m. 128-30°. 2',3,',4',6'-Tetramethoxy-chalcone, m. 74-5°, and 4,2',3',4',6'-pentamethoxychalcone, m. 88-90°, were prepare to aid in the identification of D. Similarly 3,4,2',3',4',6'hexamethoxychalcone was prepared from D with veratric adehyde, yellow, in. 127-8°, soluble in concentrated H2SO4 with intense red color. The tri-Me ether is probably 2-hydroxy-3,4,6-trimethoxyacetophenone, m. 106-8°, and gives an acetyl derivative, m 106°, and a benzoyl derivative, m. 120-2°. Condensed with veratric aldehyde it gives 2'-hydroxy-3',4',6',3,4-pentamethoxychalcone, m. 143° (identical with that of N.). B. considers the di-Me ether to be 2,6,3,4-(HO)2(MeO)2- C6HCOMe, m. 166-8°, which gives an acetyl derivative, m. 110-2°, and is probably identical with that of N. (m. 162-3°). 4 g. D with 6 g. BzOMe in 20 cc. xylene treated with 0.77 g. Na in the oil bath at about 140° gives I which is separated after cooling by treating the mixture with Et2O and dilute AcOH to decompose the Na salt formed. The Et2O solution is finally treated with 3% NaOH. This solution treated with CO2 ppts. I as yellow flocks; yellowish prisms from EtOH, m. 110-2°. 4 g. I were heated under a reflux condenser with 30-40 cc. HI (b. 126°) for 3-4 hrs., and when poured into dilute aqueous NaHSO3 separated 1,2,3-trihydroxyflavone (III), brown-yellow, m. 260° (decomposition). 4 g. III after 2 hrs. on the sand bath with 8 g. fused NaOAc + 40 g. Ac2O was cooled and the residue insol. in H2O crystallized

in the H2O mixture on standing and gave finally a diacetyl derivative of III, yellowish needles from dilute AcOH, m. 198-200°, gives the FeCl3 reaction in EtOH. On further acetyalation (7-8 hrs.) it was converted into the triacetyl derivative, white needles, m. 190-2°, gives no FeCl3 reaction. Both Ac derivs. are easily saponified in AcOH or EtOH with dilute H2SO4 or with HI (b. 126°). The Ac derivs. dissolve at first and then III begins to sep. as yellow granules. The behavior of III with reagents is described in detail, and compared with A. The EtOH solution of III treated with a little Na-Hg gives green flocks in solution This reaction is thought to be characteristic of flavones having 3 OH groups adjacent to a benzopyrone nucleus. If the 3 OH groups are adjacent to a C6H6 ring red-brown flocks are formed instead. B. points out the importance of this test if true in the identification of known and unknown compds. of this type. III was not readily methylated with MeI and Me2SO4 but with CH2N2 in Et2O gave a dimethyl ether of III as yellowish needles, m. 155-6°, which give the FeCl3reaction for OH. This result is in harmony with the accepted view that phenolic OH ortho to a side chain containing CO is more difficult to esterify. 2 g. I in 20 cc. HI (b. 126°) heated to boiling sepal. when cool on adding an aqueous solution of SO2 the tri-Me ether IV, needles from EtOH, m. 165-6°, gives no color with FeCl3.

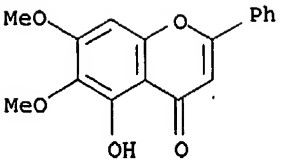
IT **491-67-8**, Baicalein
(and derivs.)
RN 491-67-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



IT **529-53-3**, Scutellarein
(constitution of)
RN 529-53-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



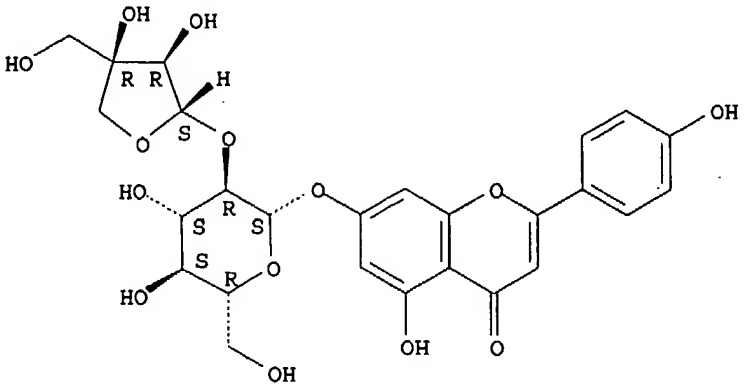
IT **740-33-0**, Flavone, 5-hydroxy-6,7-dimethoxy-
(preparation of)
RN 740-33-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-6,7-dimethoxy-2-phenyl- (9CI) (CA INDEX NAME)



L24 ANSWER 10045 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1919:7198 HCAPLUS
DOCUMENT NUMBER: 13:7198
ORIGINAL REFERENCE NO.: 13:1361c-d
TITLE: "Chrysoeriol" of "yerba santa"
AUTHOR(S): Oesterle, O. A.
CORPORATE SOURCE: Univ. Strassburg
SOURCE: Arch. Pharm. (1913), 256, 119-22
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Chrysoeriol, C16H12O6, isolated by Power and Tutin, and Tutin and Clewer, from yerba santa (cf. C. A. 3, 1523) is identical with 1,3,4'-trihydroxy-3'-methoxyflavone (Oesterle and Kueny, C. A. 12, 1553), notwithstanding the fact that Tutin and Clewer's product m. higher (337°) than that prepared by O. (324-5° decomposition). The pure acetate m. 215°, this m. p. becoming lower and indefinite on boiling the compound several hrs. with dilute alc.

L24 ANSWER 10046 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1919:1306 HCAPLUS
DOCUMENT NUMBER: 13:1306
ORIGINAL REFERENCE NO.: 13:216e-g
TITLE: Action of the potassium ferricyanide and ferric chloride reagent on alkaloids, glucosides and other plant constituents
AUTHOR(S): Palet, Luciano P. J.
SOURCE: Anales soc. quim. Argentina (1918), 6, 156-8
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB P. tested the action of the K3Fe(CN)6-Fe2(Cl)6 reagent (cf. preceding abstract) on 102 plant constituents. A positive reaction was given by the following alkaloids: apomorphine, beberine, berberine, brucine, codeine, colchicine, curarine, emetine, sparteine, erythrofleine, physostygmine, hydrastine, morphine, meconine, napeline, narcotine, pelletierine, pseudopelletierine, pereirine, sabadilline. A positive reaction was obtained with the following glucosides: adonidin, apocinin, arbutin, apiin, boldin, convalamarin, esculin, strophanthin, smilacin, floricin, globularin, graciolin, helleborin, hesperidin, sabatin, salicin, sapotoxin, siringuin. A positive reaction was obtained with the following bitter principles: aloin, cotoina verum, scoparin.
IT **26544-34-3**, Apiin
(reaction with K3Fe(CN)6-Fe2Cl6 reagent)
RN 26544-34-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 7-[(2-O-D-apio-β-D-furanosyl-β-D-glucopyranosyl)oxy]-5-hydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 10047 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1915:13951 HCAPLUS
DOCUMENT NUMBER: 9:13951
ORIGINAL REFERENCE NO.: 9:2237f-i,2238a-f
TITLE: Constitution and synthesis of scutellarein
AUTHOR(S): Bargellini, G.
CORPORATE SOURCE: Univ. Rome
SOURCE: Gazzetta Chimica Italiana (1915), 45(I), 69-80
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Scutellarein occurs in plants of the genera Scutellaria, Galeopsis and Teucrium. Goldschmidt and Zerner (C. A. 5, 1750) found it as C21H18O12, yellow needles which in 30-40% H2SO4 give by hydrolysis scutellarein (a), C15H10O6, and glucuronic acid. (a) gives yellow crystals m. about 300° (decomposition) which, heated with KOH at 200°, gives p-HOC6H4CO2H and a phenol that gives the pine reaction for phloroglucinol. Thus (a) seems to be 1,3,4-trihydroxyflavauol and since it is not identical with camphorol G. thought that (a) might be (I). G. and Z. were able to prepare the tetra-Ac (m. 235-7°), tri-Me ether (m. 189-90°), the acetyltri-Me ether (m. 167-9°) and the tetra-Me ether (m. 158-60°) derivs. Heating (a) with 12% KOH gave p-HOC6H4Ac almost quant, which shows (a) to be a flavone. The poly-OH compound formed at the same time was thought to be 1,2,3.5-C6H2(OH)4 (b) so that (a) is thus (II) or (III). (b) gives the pine chip reaction of phloroglucinol. (a) gives a green color with Ba(OH)2. B. observed that 2,5,1,3-C6H2(OH)2(OMe)2 gives a green color with alks. and became interested in the synthesis of (a). By applying v. Kostanecki's synthesis of flavones to 2,3,4,6-(MeO)4C6HAc and Me anisate plus Na, B. obtained 2,3,4,6,4'-pentamethoxybenzoylacetophenone (c) which was demethylated with HI and by loss of H2O gave the tetrahydroxyflavone which, acetylated, purified as such and. saponified, gave the flavone identical with (a). The tetra-Ac derivs. of the natural and synthetic products are identical. B. tried to obtain the derivs. in pure form but could not'do so owing to the lack of material. It was shown that (a) is either (II) or (III). It is possible that both are formed but only one has been isolated. B. oxidized apigenin (1,3,4'-trihydroxyflavone) with CrO3 (cf. Nierenstein-Wheldale, C. A. 6, 751) and obtained a red substance, probably an oxidation product (IV) (analogous to chrysone and quercetone obtained by N. and W. from chrysin and quercetin) which he hopes to convert by acetylation to the tetrahydroxyflavone derivative and thus determine whether (II) or (III) represent

the constitution of (a). 5 g. 2,3,4,6-(MeO)4C6HAc + 10 g. Me anisate + 1 g. Na gradually were heated at 125-35° 15-30 mins. The product in H2O acid with AcOH was extracted with aqueous NaOH (15 g. per 400 cc.), CO2 was passed through and a pasty red-yellow precipitate was formed. This, boiled in EtOH with animal charcoal, gave on adding H2O, 4 g. of pure yellow crystals of (c), m. 104-6°, insol. in H2O, soluble in C6H6, acetone and EtOH, gives a red color with alc. FeCl3. 2 g. (c) + 20-25 cc. HI (d. 1.7) heated under a condenser seps. the flavone. After 2 hrs. the whole is thrown into NaHSO3, filtered and washed. (a) thus obtained could not be recrystd. from organic solvents. 1 g. crude (a) + 2 g. NaOAc + 10 g. Ac2O boiled 2 hrs. separated the tetraecetyl derivative of (a), recrystd, from AcEt as white needles, m. 235-7°. 1 g. of this sapond, by heating with 10 cc. HI separated the flavone which, after treating as before, was dissolved in MeOH and gave some impure yellow-crystals. Better results were obtained by dissolving in AcOH and precipitating with H2SO4 as the sulfate which, washed on the filter, was decomposed and, recrystd. from MeOH, gave yellow laminas of (a). The tetrahydroxyflavone thus obtained showed all the characteristics of natural scutellarein as previously described by Molisch, G. and G. and Z. The sulfate is C15H10O6.H2SO4. The formation of these salts is characteristic of colored organic substances and especially flavones containing 2 adjacent OH's in the same C6H6 nucleus.

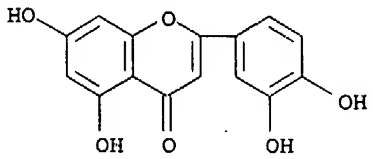
L24 ANSWER 10048 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1915:8695 HCAPLUS
DOCUMENT NUMBER: 9:8695
ORIGINAL REFERENCE NO.: 9:1311g-i,1312a-f
TITLE: Addition of auxochromes in the flavone group
AUTHOR(S): Perkin, Arthur G.; Watson, Edwin R.
CORPORATE SOURCE: Leeds, UK
SOURCE: Journal of the Chemical Society, Abstracts (1915), 107, 198-209
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C. A. 8, 1747. Derivs. of luteolin: On slowly adding 1 part luteolin tetra-Et ether (A), 3'4'-(MeO)2C6H3C.O.C6H4 (cf. C. A. 7, 2932) to 10 parts fuming HNO2 at room temperature and immediately pouring into H2O, there is precipitated tetranitroluteolin tetra-Et ether, colorless prisms, m. 196°; the mono-NO2 derivative could not be prepared Bromoluteolin tetra-Et ether perbromide, from 1 g. (A) and 2 g. Br in boiling AcOH, orange-yellow prisms, softens 157°, m., 161° (decomposition). Bromoluteolin tetra-Et ether hydrobromide (B), from (A) in AcOH with 1 mol. Br, yellow hairs with 1 AcOH, decomps. when boiled with H2O, forming bromoluteolin tetra-Et ether (C), plates, m. 183°. When 2 mols. Br and NaOAc in AcOH are used, a small amount of oxonium salt is precipitated This is filtered off, the filtrate precipitated with H2O, and the precipitate taken up in AcOH and HBr added. (B) seps. first, after which tetrabromoluteolin tetra-Et ether seps., lenticular crystals, m. 111-4°. This and (B) are also formed when the above perbromide is boiled with H2O. On adding (C) to 5 parts HNO3 (d. 1.4, NO-free), the oxonium nitrate ppts. and the mixture is warmed to 60° for 0.5 h. On cooling, bromo-6'-nitroluteolin ether (D) seps. as an oil which quickly changes to rhombs, m. 170-1°; reduced with SnCl2 and HCl it gives a crimson solution, which, on pouring into H2O, ppts. the stannichloride (crimson prisms, decomps. when boiled with H2O) of bromo-6'-aminoluteolin tetra-Et ether, yellow prisms, m. 165-9°, insol. in H2O; hydrochloride, yellow needles, with 1H2O,

becoming scarlet when anhydrous and m. 187° (decomposition), forms a crystalline diazonium chloride, which, when boiled with very dilute HCl, gives the 6'-hydroxy compound, yellow needles, m. 255°, purified through the acetate, needles, m. 270-2°. Either of these, boiled with HI (d. 1.7), remained insol., but on subsequent acetylation, gave bromo-6'-hydroxyluteolin di-Et ether triacetate, buff-colored needles, m. 213°. HI and Ac2O gave a gelatinous precipitate, which was probably the desired hydroxyluteolin, in an impure form, as it gave an impure penta-acetate, sintering above 225° and m. 250-6°. Its color is not deeper than that of luteolin. Oxidation of (D) at room temperature with alkaline KMnO4 for 1 day gave a nitro-3,4-diethoxybenzoic acid, needles, m. 145-6°. Derivs. of morin: Owing to the ease of oxidation of morin penta-Me ether (E), it was necessary to work rapidly and not to use more than 0.2 g. at a time. This was added to 2 cc. cold HNO3 (d. 1.4, NO-free) and poured into H2O as soon as all had dissolved. Nitromorin pentamethyl ether, C15H4O2(OMe)5NO3 (F), red-brown needles from alc., m. 223-5°; yield, about 50%; heated in alc. with Sn and HCl until most of the alc. is driven off, it gives the stannichloride, yellow needles, decomposed by Na2CO3, of aminomorin pentamethyl ether, plates, m. 204-5°; chloroplatinate, prisms. The corresponding hydroxy compound could not be prepared In boiling AcOH, (E) gives a brick-red per-bromide which loses Br on standing, and is converted by b. NaHSO3 into dibromomorin pentamethyl ether, rhombs, m. 263-70°; attempts to prepare a NO2 derivative failed. (F), boiled 1 h. with HI (d. 1.7), gave aminomorin hydroiodide, spherulites or platelets with 1H2O, yellow-brown. The negligible effect of the auxochromes on the colors of these compds. is explained by the fact that their effect is chiefly to widen and shift slightly toward the red the absorption band at the violet end of the spectrum, this change having little effect on the visible color.

IT **491-70-3**, Luteolin
(derivs.)

RN 491-70-3 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)



L24 ANSWER 10049 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	1912:20313 HCAPLUS
DOCUMENT NUMBER:	6:20313
ORIGINAL REFERENCE NO.:	6:2817g-i
TITLE:	Chemical Examination of the Bark of Erythrophlosum guineense
AUTHOR(S):	Power, F. B.; Salway, A. H.
SOURCE:	American Journal of Pharmacy (1835-1936) (1912), 84, 337-51 CODEN: AMJPA6; ISSN: 0093-4712
DOCUMENT TYPE:	Journal
LANGUAGE:	Unavailable

AB A quantity of the bark was completely extracted with hot EtOH and the resulting concentrate extract distilled in a current of steam but it yielded no essential oil. From the portion of the extract which was soluble in H2O the following substances were isolated: luteolin C18H1006, a small amount of an alkaloid resembling erythrophleine of Harnack, tannin, a sugar, and indefinit amorphous material. The portion of the extract insol. in H2O, consisted of a dark brown, brittle resin, representing. 13.5% of the drug and from which were obtained a phytosterol C27H44O m. 130-133°, cerotic, stearic, palmitic, oleic and linolic acids, ipuranol and luteoiln; a portion of the latter was apparently contained in the resin in the form of a glucoside. A preliminary test indicated a much larger proportion of alkaloid to be contained in the bark than could subsequently be isolated and it appeared probable that some change had taken place during the extraction

L24 ANSWER 10050 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1912:8263 HCAPLUS
DOCUMENT NUMBER: 6:8263
ORIGINAL REFERENCE NO.: 6:1297a-d
TITLE: Anthocyanin. II. Anthocyanin-like Oxidation Product of Chrysin
AUTHOR(S): Nierenstein, M.
CORPORATE SOURCE: Univ. Bristol
SOURCE: Ber. (1912), 45, 499-501
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C. A., 6, 751. Chrysone (1), from chrysin (II), glacial AcOH and CrO3; deep red needles from quinoline, not m. below 360°. In alkalies the color is blue, in concentrate H2SO4, red, changing to bluish green with a trace of (II). Acetyl derivative, red needles, m. 324-6° (decompose). With Zn dust and Ac2O, followed by dilute H2SO4 (I), gives hydroxychrysin (1,3,4-trihydroxyflavone) (III); plates, m. 304-5°. It may be sublimed. In alkalies the color is yellow, changing to brown when b. It dyes cotton the following colors with the mordants mentioned: Cr, orange; Al, yellow; Sn, light orange; Fe, blackish green. Triacetyl derivative, needles, m. 214-7°.

L24 ANSWER 10051 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1911:9669 HCAPLUS
DOCUMENT NUMBER: 5:9669
ORIGINAL REFERENCE NO.: 5:1750d-i,1751a-c
TITLE: Scutellarin
AUTHOR(S): Goldschmiedt, Guido; Zerner, Ernst
CORPORATE SOURCE: Chem. Lab. Imp.;Roy. German Univ. Prague
SOURCE: Monatshefte fuer Chemie (1911), 31, 439-91
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. Monatsh., 22, 679 (1901). The Scutellarin was obtained from Scutellaria altissima and was found to be homogeneous, except for the presence of a second substance, in very small quantity, which could not be isolated. Scutellarin is C21H18O12 not C21H20O12, as stated previously. It is a conjugated glucosidal compound; in H2O [α]D18 -14°. Barium salt, C21H16O12Ba, from BaCO3; orange-yellow. It is stable in purified air, but is quickly decompose by CO2. Methyl ester, C20H17O10CO2Me, from MeOH and H2SO4; intensely yellow, very sparingly soluble crystals which could not be purified completely, becomes gray above 200°, not m. 335°. Anhydropentacetylscutellarin, C21H11O11Ac5, from scutellarin, dry AcONa and Ac2O. When boiled with aqueous

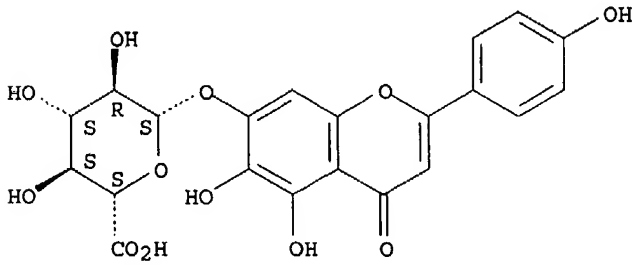
KOH, (25%), in a current of O, scutellarin gives p-hydroxyacetophenone and, if H2O2 be added to the alkaline solution, p-hydroxybenzoic acid. When suspended in H2O, treated with concentrate H2SO4 until it dissolves and then poured into H2O, it deposits scutellarein and glucuronic acid is contained in the solution Scutellarein, C15H10O6, gives the following colors on wool, with the mordants mentioned: Cr, reddish brown; Al, brownish yellow; Sn, lemon-yellow; Fe, olive-green. Hydrobromide, hydrochloride and sulfate, C15H10O6.H2SO4, intensely colored. Potassium salt, C15H9O6K, yellowish green, crystalline aggregates. Boiling HNO3 (15%) converts scutellarein into 3,5-dinitro-4-hydroxybenzoic acid. Tetraacetylscutellarein, from AcONa and Ac2O; white crystals from AcOEt, m. 235-7°. Yield, quant. Scutellarein cannot be methylated conveniently by means of Me2SO4; with KOH, MeOH and MeI it gives a mixture of tri- and tetra-Me derivs., which, however, are prepared much more readily by the action of diazomethane, followed by Me2SO4 and KOH. The 2 compds. are separated by means of dilute MeOH, in which the tetra-Me derivative is the more soluble Trimethylscutellarein, C15H7O3(OMe)3, pale yellow, rhombic plates, m. 189-90°. Yield, 65% of the scutellarein. In concentrate H2SO4 the color is greenish yellow; in alc. alkali green, changing to yellow and finally to brown; no color is produced by FeCl3. Acetyltrimethylscutellarein, from the preceding compound, AcONa and Ac2O; rhombic plates from AcOEt, m. 167-9°. Tetramethylscutellarein, C15H6O2(OMe)4, granular, slightly yellow crystals, m. 158-60°. When boiled with aqueous KOH scutellarein gives p-hydroxyacetophenone in almost quant. yield, together with a substance which could not be isolated; it resembles phloroglucinol in its color reaction with a pine splinter and it may be 1,3,4,5-tetrahydroxybenzene. The above results indicate that "scutellarein" is 1,3,4,4'- or 1,2,3,4'-tetrahydroxyflavone, formula (I) or (II) below. In dilute alc., glucuronic acid and its derivs. give a green color when treated with α-naphthol and concentrate H2SO4; with more H2O the color changes through blue to violet and even to red. The green color is regenerated by adding concentrate H2SO4. Heating produces changes similar to those brought about by H2O. These results show that the color reaction of scutellarin, described previously, is really a reaction of glucuronic acid. The reaction is also of interest in view of Molisch's sugar reaction, which consists in the production of a deep violet color when the sugar is treated with alc., α-naphthol and concentrate H2SO4.

IT **27740-01-8**, Scutellarin
(and derivs.)

RN 27740-01-8 HCAPLUS

CN β-D-Glucopyranosiduronic acid, 5,6-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-1-benzopyran-7-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 10052 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN

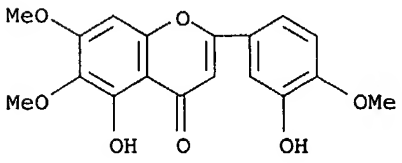
ACCESSION NUMBER: 1909:13552 HCAPLUS
DOCUMENT NUMBER: 3:13552
ORIGINAL REFERENCE NO.: 3:2485a-e
TITLE: The Constituents of Eupatorium rebaudianum, "Kaa-He-E," and Their Pharmaceutical Value
AUTHOR(S): Dieterich, K.
SOURCE: Pharmazeutische Zentralhalle fuer Deutschland (1909), 50, 435-58
CODEN: PHZEAD; ISSN: 0369-9773
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB From 8 kg. powdered leaves and stems 1850 g. dry aqueous extract were obtained. MeOH extracted from this 7% of a crude sweet substance containing over 20% ash. Its taste is intensely sweet followed by a powerful bitter after-taste. This crude sweet substance is a mixture of two compounds of similar comp. They may be separated by dissolving the crude substance in MeOH and pouring the soluble into absolute EtOH, when a bright yellow precipitate is obtained. The author names the absolute-alc.-soluble compound eupatorin and the absolute-alc.-insol. compound rebaudin. Eupatorin is soluble in EtOH, H2O, MeOH, AcOH, H2SO4, HNO3; insol. in Et2O and AcOEt; laevorotatory. Warm HCl causes turbidity-forming decompose products. A crystalline precipitate separates out from an aqueous concentrate soluble, after standing several days. If the decompose is complete the sweet taste disappears and the soluble reduces Fehling's soluble Eupatorin has no exact m. p., it softens at 114-5°. Rebaudin is similar to eupatorin but is amorphous, containing 10-11% ash, white, soluble in H2O and MeOH, insol. in absolute alc. and ether, soluble in dilute alc., HCl, glac. AcOH, H2SO4 with yellowish brown coloration. With warm HCl decompose sets in. Like the former it is laevorotatory and has no exact m. p. but softens at 107° and decomposes at 150°. Both substances are glucosides, their sweetness is about 150-180 times greater than that of sucrose. In addition to the above four other constituents were isolated: A bitter principle, soluble in alc. and ether, intensely bitter, very hygroscopic, containing no ash, m. about 50°. A vegetable wax, hard, sticky, tough and yellow, m. 57.5°; I number 32.63; acid number 10-94; ester number 86.67. A brown fatty oil having the following constants: I number 31.88-32.41 ; acid number 121.85; ester number 92.96; m. about 56°. A resin possessing the following constants: m. 63-65°; acid number 62.49-65.63; ester number 88.52-98.03.

IT **855-96-9**, Eupatorin
(preparation of)

RN 855-96-9 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-6,7-dimethoxy- (9CI) (CA INDEX NAME)



L24 ANSWER 10053 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1909:8172 HCAPLUS
DOCUMENT NUMBER: 3:8172
ORIGINAL REFERENCE NO.: 3:1523e-g
TITLE: Chemical Examination of Eriodictyon (II)
AUTHOR(S): Tutin, F.; Clewer, H. W. B.
SOURCE: Journal of the Chemical Society, Abstracts (1909), 95, 81-7
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB From the dried leaves of Eriodictyon Power and Tutin obtained eriodictyol, C15H12O5 and homoeriodictyol, C16H14O6 (Proc. Am. Pharm. Assn., 1906, 54, 352), and studied their constitution (C. A., 1, 2247, 2371; 2, 832). The authors have now obtained from the same leaves the following compounds: Xanthoeridol, C18H11O4(OH)3 (m. 258°), yellow needles. When in alc. soluble it is rendered dark brown by FeCl3. It gives triacetylxanthoeridol, C18H11O7(COCH3)3 (m. 175-6°) when treated with Ac2O. Chrysoeriol, C16H9O3(OH)3, m. above 337° AC2O. It gives triacetylchrysoeriol (211-2°) crystalline, easily undergoes partial hydrolysis. Eriodonol, C19H14O3(OH)4 (m. 209°), long yellow needles. It gives a tetraacetyleriodonol (m. 131°).

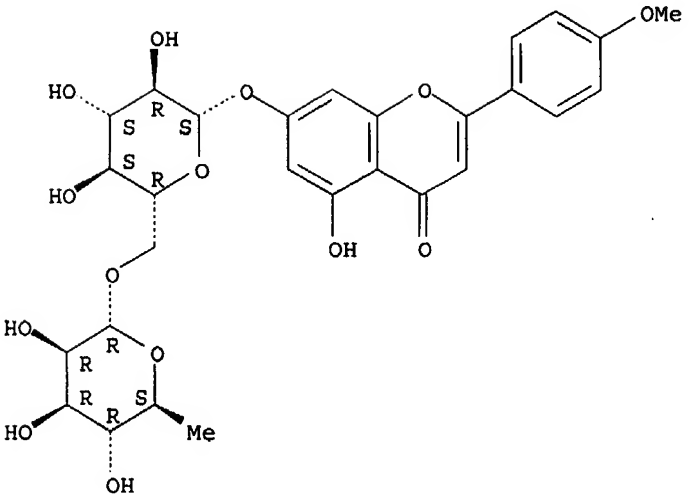
L24 ANSWER 10054 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1909:8171 HCAPLUS
DOCUMENT NUMBER: 3:8171
ORIGINAL REFERENCE NO.: 3:1523e-g
TITLE: Chemical Examination of Eriodictyon (II)
AUTHOR(S): Tutin, F.; Clewer, H. W. B.
SOURCE: Proc. Chem. Soc. (1909), 25, 12
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB From the dried leaves of Eriodictyon Power and Tutin obtained eriodictyol, C15H12O5 and homoeriodictyol, C16H14O6 (Proc. Am. Pharm. Assn., 1906, 54, 352), and studied their constitution (C. A., 1, 2247, 2371; 2, 832). The authors have now obtained from the same leaves the following compounds: Xanthoeridol, C18H11O4(OH)3 (m. 258°), yellow needles. When in alc. soluble it is rendered dark brown by FeCl3. It gives triacetylxanthoeridol, C18H11O7(COCH3)3 (m. 175-6°) when treated with Ac2O. Chrysoeriol, C16H9O3(OH)3, m. above 337° AC2O. It gives triacetylchrysoeriol (211-2°) crystalline, easily undergoes partial hydrolysis. Eriodonol, C19H14O3(OH)4 (m. 209°), long yellow needles. It gives a tetraacetyleriodonol (m. 131°).

L24 ANSWER 10055 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1908:7442 HCAPLUS
DOCUMENT NUMBER: 2:7442
ORIGINAL REFERENCE NO.: 2:1710c-i
TITLE: Syntheses in the Flavone Group
AUTHOR(S): Tambor, J.
CORPORATE SOURCE: Univ. Lab., Bern
SOURCE: Ber. (1908), 41, 787-92
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Orcacetophenone dimethyl ether (I below) forms tabular or prismatic crystals of the rhombic system, a : b : c = 0.7522 : 1 : 0.3932. 4-Methyl-2,6,2'-trimethoxybenzoylacetophenone, (MeO)2C6H2MeCOCH2COC6H4OMe, from orcacetophenone dimethyl ether, methyl methoxysalicylate and sodium. Pale red needles, m. 118° soluble in aqueous NaOH and give a blood-red color with FeCl3. 1,2'-Dihydroxy-3-methylflavone (II), from HI

and the preceding compound. Greenish yellow needles, m. 300-1°. It gives yellow solutions with concentrate H_2SO_4 and alcoholic NaOH, but does not dye mordanted cloth. Diacetyl derivative, colorless prisms, m. 108°. 1-Hydroxy-2'-methoxy-3-methylflavone, from the dihydroxy compound, MeI and KOH. Slender yellow needles, m. 156°. Sodium salt, yellow and sparingly soluble. 4-Methyl-2,6,'3-trimethoxybenzoylacetophenone, from orcacetophenone dimethyl ether and methyl m-methoxybenzoate. Light brown prisms, m. 98°. It gives a blood-red color with $FeCl_3$. 1,3'-Dihydroxy-3-methylflavone, from the preceding compound and HI. Almost colorless, silky lustrous needles, m. 227°. It gives a yellow solution with concentrate H_2SO_4 and is not a dye. Diacetyl derivative, small, yellow, rhombic prisms, m. 137°. 1-Hydroxy-3'-methoxy-3-methylflavone, small, yellow needles, m. 146°. In concentrate H_2SO_4 the solution is yellow. Sodium salt, yellow and sparingly soluble. 4-Methyl-2,6,4-trimethoxybenzoylacetophenone, from orcacetophenone dimethyl ether and methyl anisate. Colorless needles, m. 97-8°. It gives a blood-red color with $FeCl_3$. 1,4'-Dihydroxy-3-methylflavone, pale yellow, interlaced needles, m. 295°. It gives a yellow solution with concentrate H_2SO_4 and is not a dye. Diacetyl derivative, colorless, interlaced needles, m. 148-9°. 1-Hydroxy-4'-methoxy-3-methylflavone, yellow needles, m. 274°. It gives a yellow solution with concentrate H_2SO_4. Sodium salt, yellow and sparingly soluble. 4-Methyl-2,6,3',4'-tetramethoxybenzoylacetophenone, $(MeO)_2C_6H_2MeCOCH_2COC_6H_3(OMe)_2$, from orcacetophenone dimethyl ether and methyl veratrate. Colorless needles, m. 112°. It gives a blood-red color with $FeCl_3$. 1,3',4'-Trihydroxy-3-methylflavone, pale yellow, interlaced needles, m. 270°. It gives a light yellow solution with concentrate H_2SO_4. In aqueous NaOH, the color is intensely yellow. Mordanted fabrics are dyed greenish yellow. Triacetyl derivative, colorless, slender needles, m. 169°. 1-Hydroxy-3',4'-dimethoxy-3-methylflavone, yellow needles, m. 147°. It gives a yellow solution with concentrate H_2SO_4. Sodium salt, yellow and sparingly soluble.

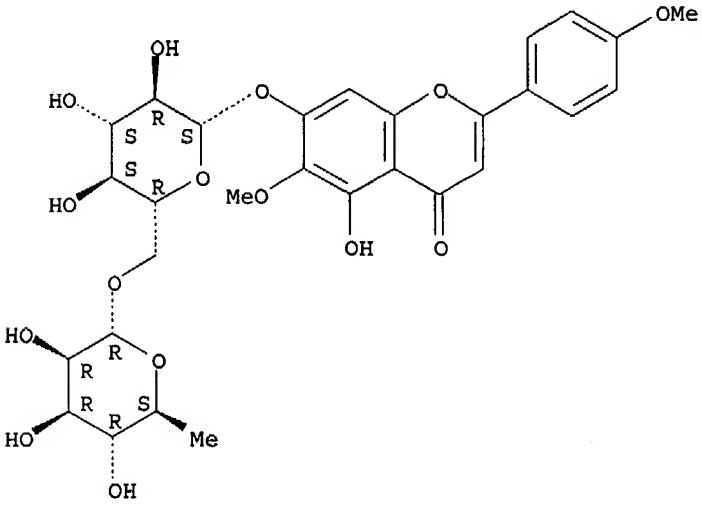
L24 ANSWER 10056 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1908:1587 HCAPLUS
DOCUMENT NUMBER: 2:1587
ORIGINAL REFERENCE NO.: 2:413g-h
TITLE: Two New Glucosides: Linarine and Pectolinarine
AUTHOR(S): Klobb, T.
SOURCE: Compt. rend. (1908), 145, 331-4
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Found in the leaves and flowers of Linaria vulgaris. Hydrolysis of pectolinarine gave a reducing sugar and two crystalline derivatives-linaric phenol, $C_{19}H_{14}O_7$, and anhydrolinaric phenol, $C_{19}H_{20}O_6$. Under the influence of alkalies pectolinarine is transformed into a β-modification which gives linaric phenol on hydrolysis. Linarine, when treated under the same conditions, gave β-linarine, which gave anhydrolinaric phenol on hydrolysis.
IT **480-36-4**, Linarin **28978-02-1**, Pectolinarin
(preparation of)
RN 480-36-4 HCAPLUS
CN 4H-1-Benzopyran-4-one, 7-[[6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-5-hydroxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 28978-02-1 HCAPLUS
CN 4H-1-Benzopyran-4-one, 7-[[6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-5-hydroxy-6-methoxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 10057 OF 10057 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1907:2207 HCAPLUS
DOCUMENT NUMBER: 1:2207
ORIGINAL REFERENCE NO.: 1:564f-i
TITLE: Synthesis of 1-Hydroxy-3-Methylflavone
AUTHOR(S): Ludwinowsky, S.; Tambor, J.
CORPORATE SOURCE: Lab. Univ. Berne
SOURCE: Ber. (1907), 39, 4037-41
DOCUMENT TYPE: Journal

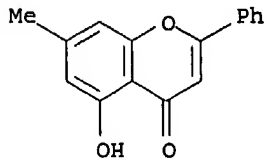
LANGUAGE: Unavailable

AB Orcinol dimethyl ether, MeC6H3(OMe)2, from orcinol and dimethyl sulphate, oily, b.120 222°. Orcacetophenone dimethyl ether, MeC6H2(OMe)2Ac, by the action of acetyl chloride and aluminum chloride on the preceding compound and also by the methylation of orcacetophenone; colorless prisms, m. 89°. 4-Methyl-2,6-dimethoxybenzoylacetophenone, MeC8H2(OMe)2COCH2Bz, by the action of ethyl benzoate and sodium on the preceding compound; tabular prisms, m. 98°-99°. It gives a blood-red color with ferric chloride. 1-Hydroxy-3-methylflavone, MeC6H2(OH), is formed when the preceding compound is boiled with hydriodic acid; slender, yellow, silky, lustrous needles, m. 143°. It is not a dye. With concentrated sulphuric acid a yellow color is formed. Sodium salt, yellow; this proves it to be a 1-hydroxyflavone and, consequently, orcacetophenone must have the formula given above and not MeC6H2(OH)2Ac. Acetyl derivative, long, colorless needles, m. 132°.

IT **33554-46-0**, Flavone, 5-hydroxy-7-methyl- (and derivs.)

RN 33554-46-0 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5-hydroxy-7-methyl-2-phenyl- (9CI) (CA INDEX NAME)



Inventors

L10 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:433756 HCAPLUS
DOCUMENT NUMBER: 140:417945
ENTRY DATE: Entered STN: 28 May 2004
TITLE: 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use
INVENTOR(S): Lahey, Thomas; Rajadhyaksha, Vithal J.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 19 pp., Cont.-in-part of U.S. Pat. Appl. 2003 69,192.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
INT. PATENT CLASSIF.:
MAIN: A61K031-7048
SECONDARY: A61K031-4178; A61K031-405; A61K031-353
US PATENT CLASSIF.: 514027000; 514456000; 514100000; 536008000; 549406000; 514397000; 514414000; 548311400; 548454000
CLASSIFICATION: 1-7 (Pharmacology)
Section cross-reference(s): 63
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004102386	A1	20040527	US 2003-652624	20030829 <--
US 2003069192	A1	20030410	US 2002-236861	20020906
US 6774142	B2	20040810		
US 2004209825	A1	20041021	US 2004-838766	20040504
WO 2005020981	A1	20050310	WO 2004-US28244	20040830

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2001-317666P	P	20010906
US 2002-407125P	P	20020830
US 2002-236861	A2	20020906
US 2003-652624	A	20030829

PATENT CLASSIFICATION CODES:

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2004102386	ICM	A61K031-7048
	ICS	A61K031-4178; A61K031-405; A61K031-353
	NCL	514027000; 514456000; 514100000; 536008000; 549406000; 514397000; 514414000; 548311400; 548454000
US 2004102386	ECLA	A61K031/352; A61K031/353; C07D311/30; C07D311/32 <--
US 2003069192	ECLA	A61K031/352; A61K031/353; C07D311/30; C07D311/32
US 2004209825	ECLA	A61K031/352; A61K031/353; C07D311/30; C07D311/32

OTHER SOURCE(S): MARPAT 140:417945
ABSTRACT:

The invention discloses 3-deoxyflavonoid compds. and methods for inhibiting T-cell activity and treating diseases and disorders (e.g. autoimmune disorders, inflammatory disorders, diabetes, ALS, MS, rheumatoid arthritis, etc.). In some cases the efficacy and/or duration of action of luteolin and/or other 3-deoxyflavonoid compds. may be increased by administering such compds. along with rutin, a rutin congener and/or a rutin derivative Also, in some cases, first pass metabolism of luteolin or other 3-deoxyflavonoids may be avoided by administering such compds. by parenteral routes (e.g., routes wherein absorption occurs at sites other than the stomach or intestinal mucosa, such as sublingual, buccal, intranasal, injection, etc.).

SUPPL. TERM: deoxyflavonoid T lymphocyte activation inhibition therapeutic antiinflammatory antidiabetic antirheumatic; luteolin rutin T lymphocyte activation inhibition therapeutic

INDEX TERM: Antidiabetic agents
Autoimmune disease
Diabetes mellitus
Human
Immunosuppressants
Multiple sclerosis
Nervous system agents
T cell (lymphocyte)
(3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Flavonoids
ROLE: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Cell activation
(T cell; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: T cell (lymphocyte)
(activation; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Nervous system, disease
(amyotrophic lateral sclerosis; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Drug delivery systems
(buccal; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: T cell (lymphocyte)
(cytotoxic; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Muscle, disease
(fibromyalgia; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Drug metabolism
(first-pass metabolism; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Drug delivery systems
(injections; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Diabetes mellitus
(insulin-dependent; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Drug delivery systems
(nasal; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Diabetes mellitus
(non-insulin-dependent; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Drug delivery systems
(oral; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Ion channel blockers
(potassium, Kv1.3 channel; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Drug delivery systems
(rectal; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Drug delivery systems
(sublingual; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Drug delivery systems
(tablets; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Drug delivery systems
(transdermal; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: Drugs
(veterinary; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

INDEX TERM: **153-18-4**, Rutin **153-18-4D**, Rutin, derivs. and congeners **446-72-0**, Genistein **486-66-8**, Daidzein **491-70-3**, Luteolin **501445-13-2** **501445-14-3** **501445-15-4** **501445-16-5** **501445-17-6** **501445-18-7** **501445-19-8**
ROLE: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

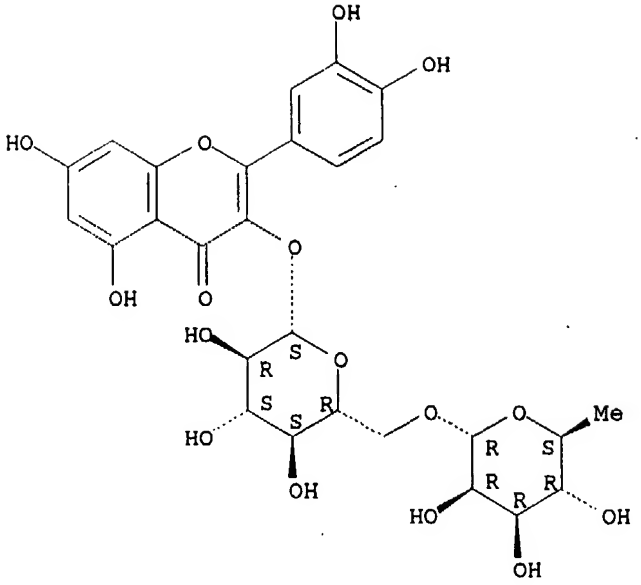
INDEX TERM: **50-99-7**, D-Glucose, biological studies
ROLE: BSU (Biological study, unclassified); BIOL (Biological study)
(stabilization of blood levels of; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

IT **153-18-4**, Rutin **153-18-4D**, Rutin, derivs. and congeners **446-72-0**, Genistein **486-66-8**, Daidzein **491-70-3**, Luteolin **501445-13-2** **501445-14-3** **501445-15-4** **501445-16-5** **501445-17-6** **501445-18-7** **501445-19-8**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)

RN 153-18-4 HCAPLUS

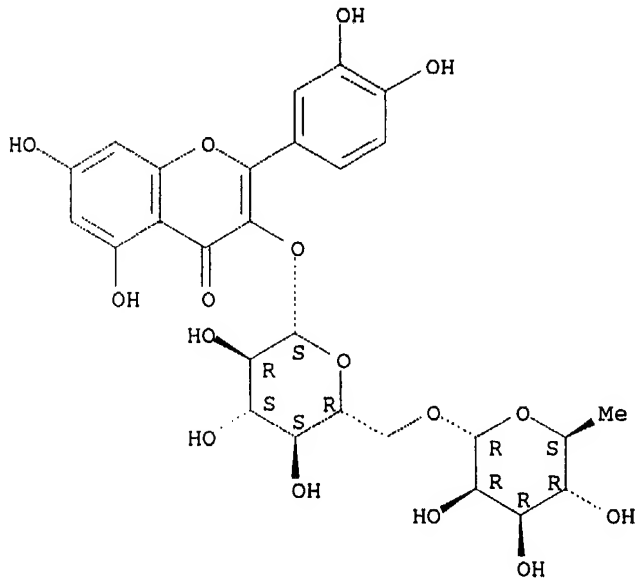
CN 4H-1-Benzopyran-4-one, 3-[[6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



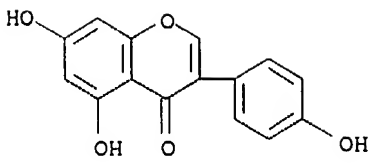
RN 153-18-4 HCAPLUS
CN 4H-1-Benzopyran-4-one, 3-[[6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

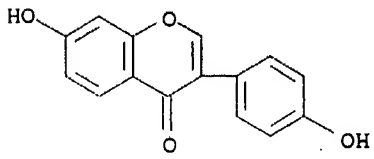


RN 446-72-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX

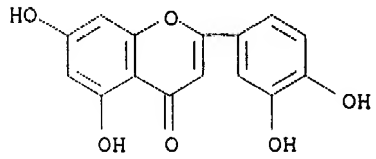
NAME)



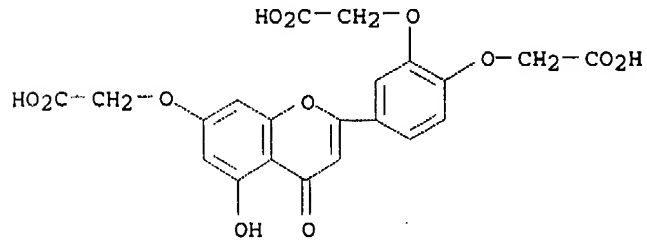
RN 486-66-8 HCAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



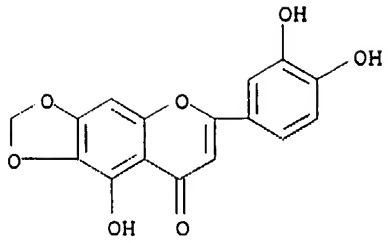
RN 491-70-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)



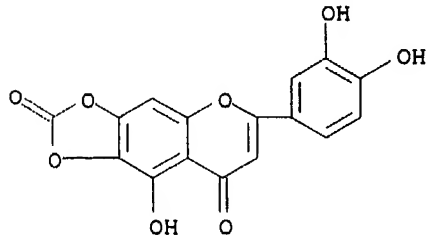
RN 501445-13-2 HCAPLUS
CN Acetic acid, 2,2'-[[4-[7-(carboxymethoxy)-5-hydroxy-4-oxo-4H-1-benzopyran-2-yl]-1,2-phenylene]bis(oxy)]bis- (9CI) (CA INDEX NAME)



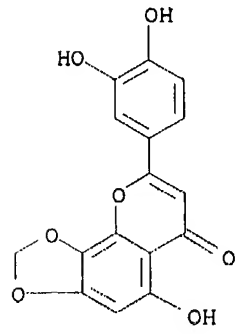
RN 501445-14-3 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-8-one, 6-(3,4-dihydroxyphenyl)-9-hydroxy- (9CI) (CA INDEX NAME)



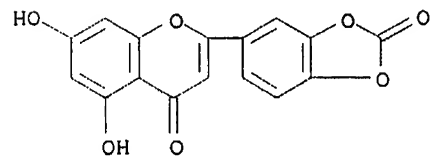
RN 501445-15-4 HCAPLUS
CN 8H-1,3-Dioxolo[4,5-g][1]benzopyran-2,8-dione, 6-(3,4-dihydroxyphenyl)-9-hydroxy- (9CI) (CA INDEX NAME)



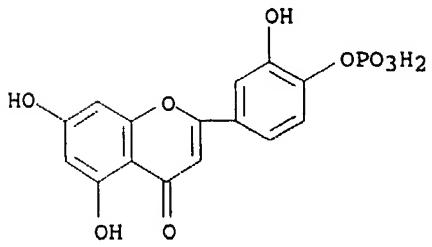
RN 501445-16-5 HCAPLUS
CN 6H-1,3-Dioxolo[4,5-h][1]benzopyran-6-one, 8-(3,4-dihydroxyphenyl)-5-hydroxy- (9CI) (CA INDEX NAME)



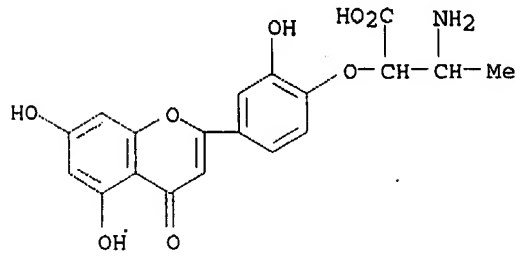
RN 501445-17-6 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-(2-oxo-1,3-benzodioxol-5-yl)- (9CI) (CA INDEX NAME)



RN 501445-18-7 HCAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-[3-hydroxy-4-(phosphonooxy)phenyl]- (9CI) (CA INDEX NAME)

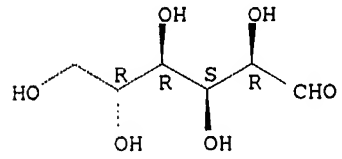


RN 501445-19-8 HCAPLUS
CN Butanoic acid, 3-amino-2-[4-(5,7-dihydroxy-4-oxo-4H-1-benzopyran-2-yl)-2-hydroxyphenoxy]- (9CI) (CA INDEX NAME)

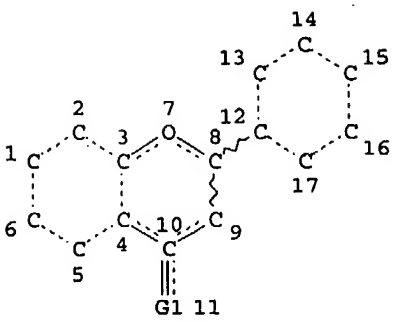


IT **50-99-7**, D-Glucose, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(stabilization of blood levels of; 3-Deoxyflavonoid inhibition of T-lymphocyte activation, and therapeutic use)
RN 50-99-7 HCAPLUS
CN D-Glucose (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d que l32
L1 STR



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VAR G1=O/S
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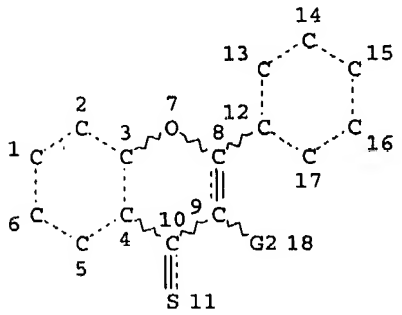
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L2 36287 SEA FILE=REGISTRY SSS FUL L1
L30 STR



VAR G2=H/F
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L31 111 SEA FILE=REGISTRY SUB=L2 SSS FUL L30
L32 67 SEA FILE=HCAPLUS ABB=ON PLU=ON L31

=> d l32 ibib ab hitstr 1-67

L32 ANSWER 1 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:825133 HCAPLUS
DOCUMENT NUMBER: 141:332051
TITLE: Preparation of substituted chromen-4-one oximes as inhibitors of protein kinases
INVENTOR(S): Green, Jeremy; Aronov, Alex; Pierce, Albert C.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 47 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004198750	A1	20041007	US 2004-808678	20040325
WO 2004092154	A1	20041028	WO 2004-US9145	20040325

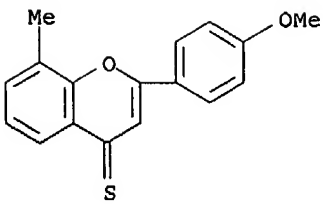
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-460042P P 20030403
OTHER SOURCE(S): MARPAT 141:332051

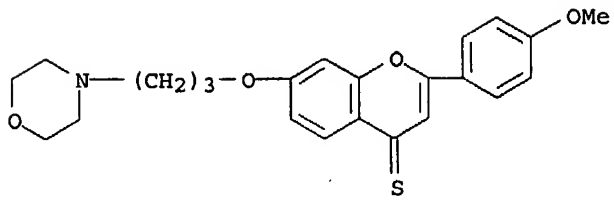
AB The title compds. [I; R1 = LmR, LmAr1, LmCy1; L = S, O, NR, alkylidene wherein up to two non-adjacent methylene units of L are optionally replaced by S, O, CO, etc.; m = 0-1; Ar1 = (un)substituted 5-7 membered monocyclic or 8-10 membered bicyclic ring having 0-5 heteroatoms; Cy1 = (un)substituted 3-7 membered (un)saturated monocyclic ring having 0-3 heteroatoms or 8-10 membered (un)saturated bicyclic ring having 0-5 heteroatoms; R = H, alkyl; R2 = H, CN, SR, OR, etc.; T = N, CR3; A1-A3 = N, CR4; provided that no more than two of T, A1-A3 are N atom; R3 = H, halo, NO2, etc.; R4 = halo, NO2, CN, etc.; with provisos], useful as inhibitors of protein kinases, were prepared E.g., a 2-step synthesis of 2-(4-methoxyphenyl)-8-methylchromen-4-one oxime, starting from 8-methyl-4'-methoxyflavone, was given. The exemplified compds. I were tested and found to inhibit CDK-2, cMET, GSK-3, SYK, ZAP-70, FLT-3, JAK-3, p70S6K, TAK-1, and IRAK-4. The invention also provides pharmaceutically acceptable compns. comprising said compds. I and methods of using the compns. in the treatment of various disease, conditions, or disorders.

IT **769949-18-0P**, 2-(4-Methoxyphenyl)-8-methylchromene-4-thione
769949-21-5P, 2-(4-Methoxyphenyl)-7-(3-(morpholin-4-yl)propoxy)chromen-4-thione
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted chromen-4-one oximes as inhibitors of protein kinases)

RN 769949-18-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methoxyphenyl)-8-methyl- (9CI) (CA INDEX NAME)



RN 769949-21-5 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methoxyphenyl)-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)



L32 ANSWER 2 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:765642 HCAPLUS
DOCUMENT NUMBER: 142:49162
TITLE: Modulation of CYP19 activity: small change of flavonoid structure results in inhibitor - stimulator transition
AUTHOR(S): Hodek, P.; Provaznikova, D.; Smrcek, S.; Istvankova, B.; Stiborova, M.
CORPORATE SOURCE: Department of Biochemistry, Faculty of Science, Charles University, Prague, Czech Rep.
SOURCE: Cytochromes P450: Biochemistry, Biophysics and Drug Metabolism, International Conference on Cytochromes P450, 13th, Prague, Czech Republic, June 29-July 3, 2003 (2003), Meeting Date 2003, 177-182. Editor(s): Anzenbacher, Pavel; Hudecek, Jiri. Monduzzi Editore: Bologna, Italy.
CODEN: 69FTSZ; ISBN: 88-323-3142-X
DOCUMENT TYPE: Conference; (computer optical disk)
LANGUAGE: English

AB Flavonoids, extensively studied as potential anti-cancer agents, resemble the steroid skeleton and thus effectively inhibit aromatase (CYP19). To elucidate the role of C4 oxo-group of the flavonoid moiety for the inhibition, we derivatized this position in the most effective aromatase flavonoid inhibitor, 7,8-benzoflavone (ANF) with substitution for sulfur. The resulting thio-analog of ANF (SANF) showed a stimulatory effect on human placental CYP19. Formation of estrone from androstendione in human placental microsomes as well as dibenzylfluoresceine metabolism in microsomes containing human recombinant CYP19 were increased to 150-160% of control. In addition, dibenzylfluoresceine metabolism in human placental microsomes was almost doubled.

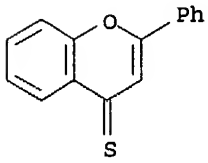
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:807792 HCAPLUS
DOCUMENT NUMBER: 140:391166
TITLE: Product class 4: benzopyranones and benzopyranthiones
AUTHOR(S): Williams, A. C.; Camp, N.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2003), 14, 347-638
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

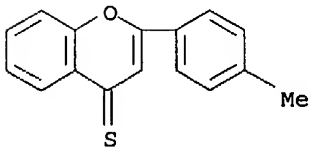
AB A review. Methods for preparing 2H-1-benzopyran-2-ones, 4H-1-benzopyran-4-ones, 1H-2-benzopyran-1-ones, 6H-dibenzo[b,d]pyran-6-ones, 9H-xanthenones and their corresponding thione analogs as well as 3H-2-benzopyran-3-ones are surveyed. Synthetic methods include ring closure, ring transformation, aromatization and substituent modification reactions.

IT **5465-04-3P 16074-59-2P 155938-47-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(review of preparation of benzopyranones and benzopyranthiones via ring closure, ring transformations, aromatization and substituent modifications)

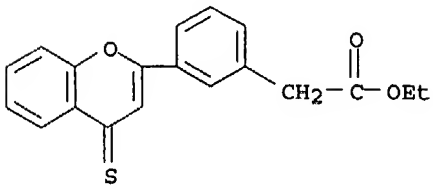
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



RN 16074-59-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 155938-47-9 HCAPLUS
CN Benzeneacetic acid, 3-(4-thioxo-4H-1-benzopyran-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)



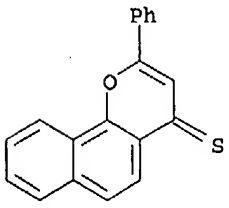
REFERENCE COUNT: 1083 THERE ARE 1083 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 4 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:592763 HCAPLUS
DOCUMENT NUMBER: 139:291912
TITLE: Singlet and triplet state properties of substituted flavothiones
AUTHOR(S): Aloisi, Gian G.; Latterini, Loredana; Macanita, Antonio L.; Becker, Ralph S.; Elisei, Fausto
CORPORATE SOURCE: Dipartimento di Chimica, Universita di Perugia, Perugia, Italy
SOURCE: Physical Chemistry Chemical Physics (2003), 5(16), 3464-3469
CODEN: PPCPFQ; ISSN: 1463-9076
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

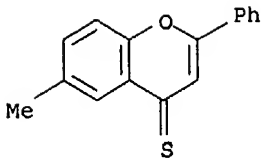
AB The properties of the singlet and triplet excited states of some substituted flavothiones in different solvents are presented. Steady-state and pulsed techniques were used to characterize the emitting S2 state ($\pi \rightarrow \pi^*$ in nature, kF $\approx$ 107 s-1) in terms of fluorescence quantum yields (.apprx.10-4) and lifetimes (in the picosecond range). As for other flavothiones, no emission was observed from the lowest excited S1 state of n,π^* nature. Information on the state order and on the oscillator strengths of singlet-singlet transitions were obtained by semiempirical calcns. The lowest excited triplet states (T1) were characterized by laser flash photolysis in terms of absorption spectra, formation quantum yields, decay lifetimes and molar absorption coeffs. The interaction of T1 with mol. oxygen leads to singlet oxygen with quantum yield generally high ($\Phi\Delta$.apprx.0.55). The study of triplet properties allowed information on the mechanism of intersystem crossing and on the triplet nature of the various flavothiones to be obtained.

IT **14882-98-5**, 7,8-Benzothioflavone **140885-77-4** **171119-01-0** **422564-16-7**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(singlet and triplet state properties of substituted flavothiones)

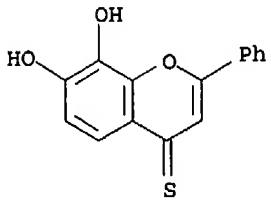
RN 14882-98-5 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-phenyl- (8CI, 9CI) (CA INDEX NAME)



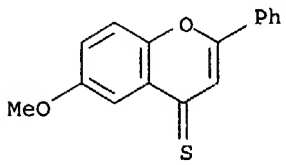
RN 140885-77-4 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



RN 171119-01-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7,8-dihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 422564-16-7 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-methoxy-2-phenyl- (9CI) (CA INDEX NAME)



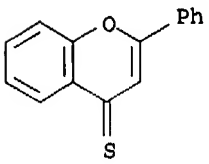
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 5 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:61905 HCAPLUS
DOCUMENT NUMBER: 138:392921
TITLE: Photochemistry of flavothione and hydroxyflavothiones: mechanisms and kinetics
AUTHOR(S): Macanita, Antonio L.; Elisei, Fausto; Aloisi, Gian Gaetano; Ortica, Fausto; Bonifacio, Vasco; Dias, Antonio; Leitao, Emilia; Caldeira, Maria Joao; Maycock, Christopher D.; Becker, Ralph S.
CORPORATE SOURCE: Instituto de Tecnologia Quimica e Biologica, Oeiras, 2800, Port.
SOURCE: Photochemistry and Photobiology (2003), 77(1), 22-29
CODEN: PHCBAP; ISSN: 0031-8655
PUBLISHER: American Society for Photobiology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors present a detailed study of the mechanism of photochem. and thermal reactions, as well as of the kinetics of flavothione (FLT) in ethanol. The authors analyzed how the hydroxy-substitution pattern of FLT influenced both the kinetics and the mechanism relative to the parent FLT. The authors show that the primary photochem. reaction of FLT in the absence of oxygen is hydrogen (H)-atom abstraction from the solvent by way

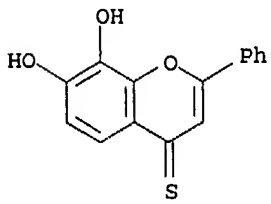
of the excited triplet state of FLT. Several products result from thermal reactions of the resulting semireduced FLTH• radical, including more than one dimer. A full mechanism is proposed, and the relevant rate consts. are evaluated. On the other hand, in the presence of oxygen and a low concentration of FLT, the authors found that the principal photoproduct is the parent flavone (FL). The reaction leading to photoxidn. is not via 1O2 attacking a thione, but instead, it is via a reaction of the FLTH• radical with ground state oxygen. The kinetic data also demonstrate that the relative values of concns. of reactants and the rate consts. of the reactions can control the dominance of one mechanism over others. The authors also have examined the photochem. mechanisms and kinetics for several hydroxyflavothiones (n-OHFLT) and compared them with FLT itself. The authors have found that the photochem. mechanism radically changes depending on the positions of substitution. These differences are directly related to the ordering of the excited states of the n-OHFLT. Specifically, FLT with lowest 3n,π* states (FLT, 6-hydroxyflavothione, 7-hydroxyflavothione and 7,8-dihydroxyflavothione) efficiently abstract H atoms to give the semireduced radical of the thione. The radical can (1) dimerize to form two different dimers; (2) react with oxygen to produce the parent FL; and (3) recombine with the solvent radical to yield the original FLT. In contrast, FLT with lowest 3π,π* states (3-hydroxyflavothione, 3,6-dihydroxyflavothione and 3,7-dihydroxyflavothione) behave as photosensitizers of oxygen to form singlet oxygen, which then reacts with the ground state of the substituted FLT. Finally, when T2(π,π*) is above S1(n,π*), as for 5-hydroxyflavothione and 5,7-dihydroxyflavothione, both the S1(n,π*) → T1(n,π*) intersystem crossing and photodegrdn. are inefficient.

IT **5465-04-3 171119-01-0 284684-02-2 284684-03-3**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(mechanisms and kinetics of photochem. reactions of flavothione and hydroxyflavothiones in presence and absence of oxygen)

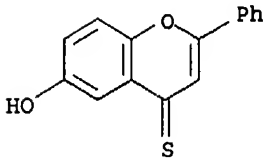
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



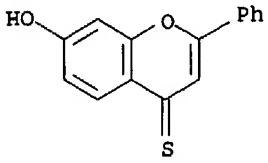
RN 171119-01-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7,8-dihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 284684-02-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 284684-03-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



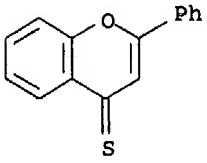
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 6 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:203460 HCAPLUS
DOCUMENT NUMBER: 136:365876
TITLE: Photobiological properties of hydroxy-substituted flavothiones
AUTHOR(S): Borges, Marta; Romao, Ana; Matos, Olivia; Marzano, Christine; Caffieri, Sergio; Becker, Ralph S.; Macanita, Antonio L.
CORPORATE SOURCE: Instituto de Tecnologia Quimica e Biologica, Oeiras, 2800, Port.
SOURCE: Photochemistry and Photobiology (2002), 75(2), 97-106
CODEN: PHCBAP; ISSN: 0031-8655
PUBLISHER: American Society for Photobiology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Flavothione (FT) and a series of 18 hydroxy- and methoxy-substituted flavothiones were screened for photobiol. activity. The 5-hydroxy-substituted compds. (group 3) and the methoxy-substituted flavothiones were inactive. FT and the remaining hydroxy-substituted compds., all displayed photobiol. activity. Among these, the 3-hydroxy-substituted compds. (group 2) were the most efficient photosensitizers overall in spite of their concurrent fast photodegrdn. FT and all other hydroxyflavothiones, not substituted in the 3- or 5-positions (group 1), were inefficient compared with group 2. Detailed photobiol. tests were carried out for four flavothiones of groups 1 and 2. The biol. tests included fungi, several strains of Escherichia coli, Salmonella typhimurium and mammalian cells. In addition, the ability of these flavothiones to perform lipid peroxidn. was evaluated. FT and 6-hydroxyflavothione (group 1) induce DNA damage via H-atom abstraction from the lowest n, π^* triplet state of the thione (oxygen independent). For 3-hydroxy and 3,6-dihydroxyflavothione (group 2), both DNA and the membrane are targets. The mechanism likely involves both energy transfer

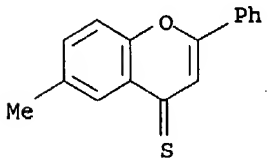
and electron transfer from the lowest π, π* triplet state to oxygen, to form singlet oxygen and the superoxide anion. Some of these compds. could be considered as models for environmentally safe photopesticides.

IT **5465-04-3 140885-77-4 171119-01-0**
284684-01-1 284684-02-2 284684-03-3
422564-10-1 422564-11-2 422564-12-3
422564-13-4 422564-15-6 422564-16-7
422564-17-8 422564-18-9
RL: ADV (Adverse effect, including toxicity); AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(photobiol. properties of hydroxy-substituted flavothiones)

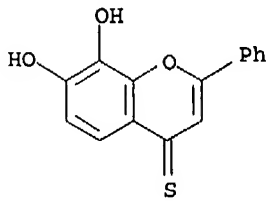
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



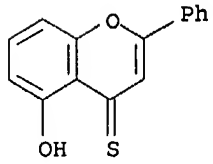
RN 140885-77-4 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



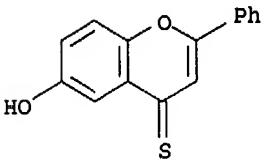
RN 171119-01-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7,8-dihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



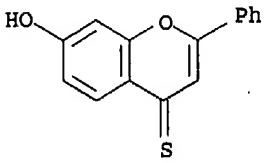
RN 284684-01-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 5-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



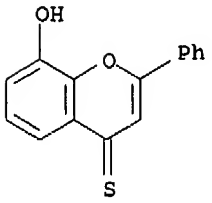
RN 284684-02-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



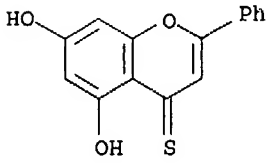
RN 284684-03-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



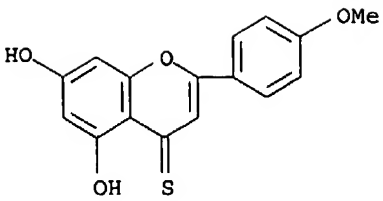
RN 422564-10-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 8-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 422564-11-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 5,7-dihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 422564-12-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 5,7-dihydroxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 422564-13-4 HCAPLUS
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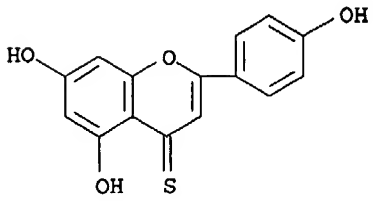

RN 422564-15-6 HCAPLUS
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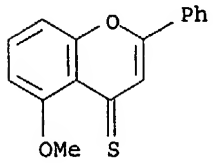
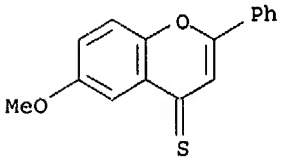
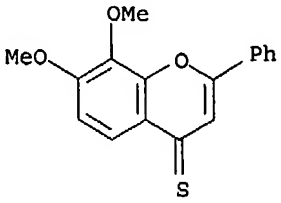


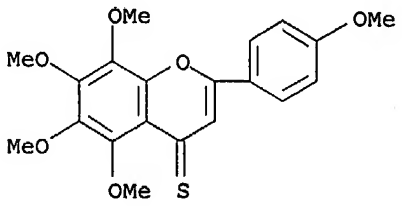
RN 422564-16-7 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-methoxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 422564-17-8 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7,8-dimethoxy-2-phenyl- (9CI) (CA INDEX NAME)

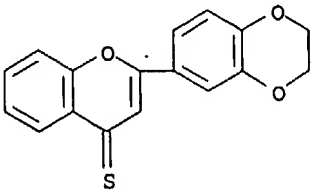


RN 422564-18-9 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 5,6,7,8-tetramethoxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

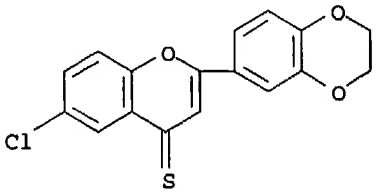


REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 7 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:175148 HCAPLUS
DOCUMENT NUMBER: 134:326293
TITLE: Synthetic analogs of naturally occurring flavolignans. X. Reaction of flavones and their thioderivatives with hydroxylamine
AUTHOR(S): Aitmambetov, A.; Khilya, V. P.; Kubzheterova, A.
CORPORATE SOURCE: Complex Institute of Natural Sciences, Karakalpak Division, Academy of Sciences of the Republic of Uzbekistan, Nukus, 742000, Uzbekistan
SOURCE: Chemistry of Natural Compounds (Translation of Khimiya Prirodnykh Soedinenii) (2000), 36(1), 47-50
CODEN: CHNCA8; ISSN: 0009-3130
PUBLISHER: Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:326293
AB 1,3-Benzodioxoles, 1,4-benzodioxanes, and 1,5-benzodioxepanes are flavone analogs that hydroxylamine recyclizes into derivs. of 5-(2-hydroxyphenyl)isoxazoles. They react with thio derivs. with retention of the pyrone ring and formation of oximes. Their structures are proven using PMR spectra.
IT **202914-92-9 202914-94-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of hydroxylamine with flavones and their thio derivs.)
RN 202914-92-9 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(2,3-dihydro-1,4-benzodioxin-6-yl)- (9CI) (CA INDEX NAME)



RN 202914-94-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-chloro-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-(9CI) (CA INDEX NAME)



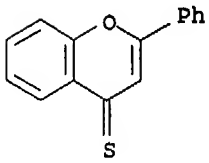
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 8 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:372202 HCAPLUS
DOCUMENT NUMBER: 133:119982
TITLE: Photophysical Properties of Hydroxy-Substituted Flavothiones
AUTHOR(S): Elisei, Fausto; Lima, Joao C.; Ortica, Fausto; Aloisi, Gian G.; Costa, Manuela; Leitao, Emilia; Abreu, Isabel; Dias, Antonio; Bonifacio, Vasco; Medeiros, Jorge; Macanita, Antonio L.; Becker, Ralph S.
CORPORATE SOURCE: Dipartimento di Chimica, Universita di Perugia, Perugia, 2800, Italy
SOURCE: Journal of Physical Chemistry A (2000), 104(25), 6095-6102
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Flavothione and a number of synthesized hydroxy- (mono- and di-) substituted flavothiones have been thoroughly examined, particularly regarding their absorption, emission, photophys. (triplet yields and lifetimes), and oxygen-photosensitizing characteristics. These were all studied as a function of the nature of the solvent (four), which was particularly critical in terms of aiding in determining the energy and configurational nature of the lowest triplet state as well as the mechanism of intersystem crossing. Theor. calcns. were also performed. Both the location and number of hydroxyl groups have a substantial impact on the nature of the lowest excited triplet state as well as on the relative location of the two lowest excited singlet and triplet states. These in turn affect the magnitude and even the existence of triplet-state occupation as well as the ability to sensitize oxygen (to singlet oxygen). Three groups of compds. exist as characterized by the configurational nature of the triplet and the mechanism of intersystem crossing, or the essential absence of intersystem crossing altogether. The quantum yield of singlet oxygen formation is

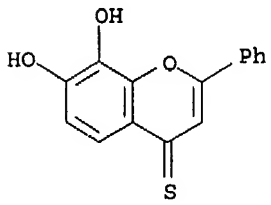
high for one group where the T(π, π^*) state is lowest and generally high in another group where the T(n, π^*) state is lowest, except in ethanol where competitive H-atom abstraction occurs. The potential of all hydroxy compds. as photosensitizers is evaluated.

IT **5465-04-3 171119-01-0**, 4H-1-Benzopyran-4-thione, 7,8-dihydroxy-2-phenyl- **284684-01-1 284684-02-2 284684-03-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(absorption, emission, photophys. (triplet yields and lifetimes), and oxygen-photosensitizing characteristics of hydroxy-substituted flavothiones)

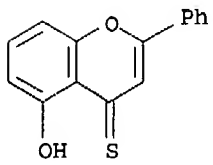
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



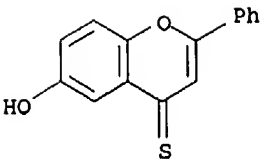
RN 171119-01-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7,8-dihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



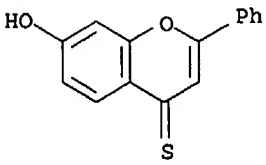
RN 284684-01-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 5-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 284684-02-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)

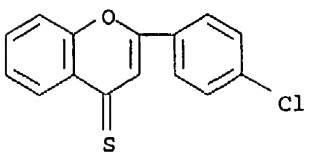


RN 284684-03-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7-hydroxy-2-phenyl- (9CI) (CA INDEX NAME)

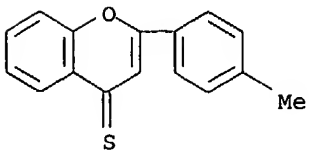


REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

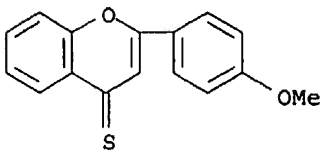
L32 ANSWER 9 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:749455 HCAPLUS
DOCUMENT NUMBER: 132:122483
TITLE: An efficient procedure for the preparation of 4-thioflavones by the reaction of flavones with Lawesson's reagent
AUTHOR(S): Levai, Albert
CORPORATE SOURCE: Department of Organic Chemistry, Lajos Kossuth University, Debrecen, H-4010, Hung.
SOURCE: Heterocyclic Communications (1999), 5(5), 419-422
CODEN: HCOMEX; ISSN: 0793-0283
PUBLISHER: Freund Publishing House Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:122483
AB A simple and convenient procedure has been worked out for the preparation of 4-thioflavones I (R = 3-Me, 2,4-Cl2, 4-NO2, etc., X = S) by the reaction of flavones I (X = O) with Lawesson's reagent under reflux for 3 h.
IT **16074-52-5P 16074-59-2P 82340-44-1P 84212-79-3P 93321-88-1P 256464-67-2P 256464-68-3P 256464-69-4P 256464-70-7P 256464-71-8P 256464-72-9P 256464-73-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of thioflavones by sulfuration of flavones with Lawesson's reagent)
RN 16074-52-5 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



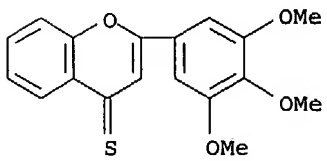
RN 16074-59-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



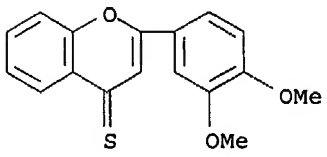
RN 82340-44-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



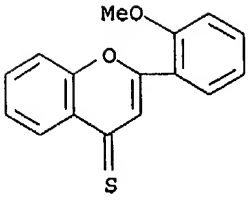
RN 84212-79-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



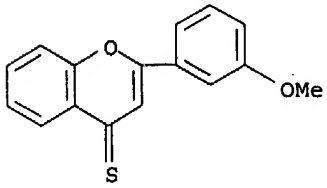
RN 93321-88-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



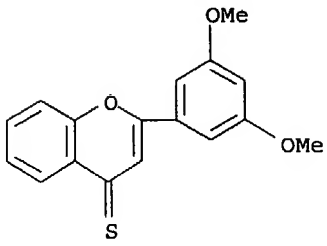
RN 256464-67-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



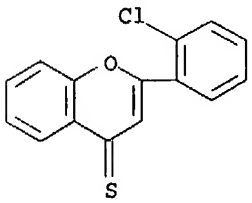
RN 256464-68-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)



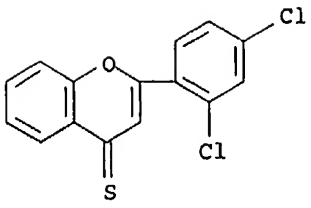
RN 256464-69-4 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



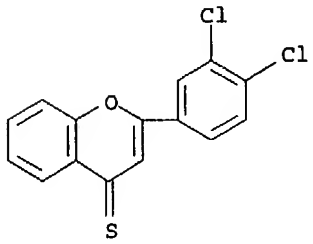
RN 256464-70-7 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



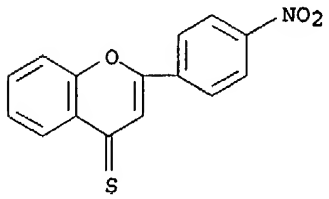
RN 256464-71-8 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(2,4-dichlorophenyl)- (9CI) (CA INDEX NAME)



RN 256464-72-9 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(3,4-dichlorophenyl)- (9CI) (CA INDEX NAME)



RN 256464-73-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



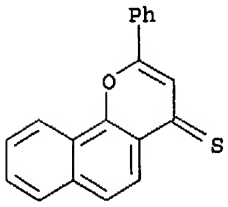
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 10 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:479842 HCAPLUS
DOCUMENT NUMBER: 131:257163
TITLE: Triplet states of aromatic thioketones supported on cellulose
AUTHOR(S): Sikorski, M.; Wilkinson, F.; Bourdelande, J. L.; Gonzalez Moreno, R.; Steer, R. P.
CORPORATE SOURCE: Department of Chemistry, University of Saskatchewan, Saskatoon, SK, Can.
SOURCE: Physical Chemistry Chemical Physics (1999), 1(15), 3639-3645
CODEN: PPCPFQ; ISSN: 1463-9076
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Diffuse-reflectance and emission and transient diffuse-reflectance measurements of the spectra and decay kinetics of several aromatic thiones

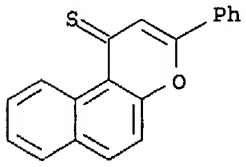
supported on cellulose provided information concerning the 2nd excited singlet state, S2, the lowest triplet state, T1, and transient chemical intermediates formed when these materials are excited in the near UV. Thermally activated delayed fluorescence from the lowest excited singlet state, S1, is a minor component of the emission at room temperature, but not at 77 K because back-intersystem crossing is eliminated, resulting in a substantial lengthening of the triplet lifetime. At room temperature, the triplet states have lifetimes of the order of μs and the chemical intermediates have lifetimes of hundreds of μs. Comparisons of the triplet spectra in polar and nonpolar media with those on cellulose show that T1 is of π,π* configuration on the solid support, as expected if the thione is adsorbed in a polar microenvironment. The triplet decay times, but not the spectra, indicate that the thiones are in different microenvironments when they are adsorbed from MeCN compared with MeOH. The latter have decay times characteristic of single mols.; the former may indicate the thiones are adsorbed as aggregates. Singlet mol. oxygen, O2(1Δg), observed directly by transient emission at 1270 nm, is formed with near unit efficiency from the thione triplets in fluid MeCN solution, but O2 has no measurable effect on the triplet spectra and decay times when the thione is supported on cellulose.

IT **14882-98-5**, 4H-Naphtho[1,2-b]pyran-4-thione, 2-phenyl-
139448-82-1, 1H-Naphtho[2,1-b]pyran-1-thione, 3-phenyl-
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(triplet states of aromatic thioketones supported on cellulose)

RN 14882-98-5 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-phenyl- (8CI, 9CI) (CA INDEX NAME)



RN 139448-82-1 HCAPLUS
CN 1H-Naphtho[2,1-b]pyran-1-thione, 3-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

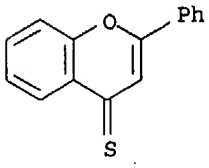
L32 ANSWER 11 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:469261 HCAPLUS
DOCUMENT NUMBER: 131:228267
TITLE: Microwave-Accelerated Solvent-Free Synthesis of Thioketones, Thiolactones, Thioamides, Thionoesters,

and Thioflavonoids
AUTHOR(S): Varma, Rajender S.; Kumar, Dalip
CORPORATE SOURCE: Department of Chemistry, Texas Research Institute for Environmental Studies (TRIES), Huntsville, TX, 77341-2117, USA
SOURCE: Organic Letters (1999), 1(5), 697-700
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:228267

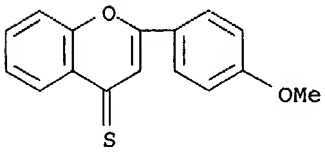
AB An expeditious, solvent-free, and high yield conversion of ketones, flavones, isoflavones, lactones, amides, and esters to the corresponding thio analogs is described utilizing Lawesson's reagent in a process that circumvents the use of dry solvents and excess of the reagent.

IT **5465-04-3P 82340-44-1P 244107-94-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(microwave-accelerated solvent-free synthesis of thioketones, thiolactones, thioamides, thionoesters, and thioflavonoids)

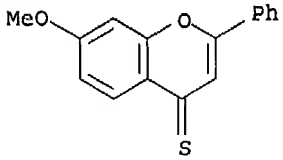
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



RN 82340-44-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 244107-94-6 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7-methoxy-2-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

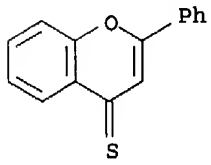
L32 ANSWER 12 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:221085 HCAPLUS
DOCUMENT NUMBER: 130:311380
TITLE: Solventless regeneration of ketones from thioketones using clay supported nitrate salts and microwave irradiation
AUTHOR(S): Varma, Rajender S.; Kumar, Dalip
CORPORATE SOURCE: Department of Chemistry and Texas Research Institute for Environmental Studies, Sam Houston State University, Huntsville, TX, 77341-2117, USA
SOURCE: Synthetic Communications (1999), 29(8), 1333-1340
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:311380

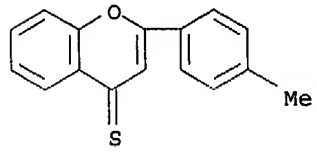
AB Thioketones are readily converted into the corresponding ketones under solvent-free conditions using clayfen or clayan in a process that is accelerated by microwave irradiation

IT **5465-04-3 16074-59-2 82340-44-1**
223594-07-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(solventless regeneration of ketones from thioketones using clay supported nitrate salts and microwave irradiation)

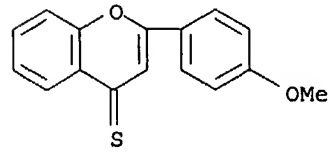
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



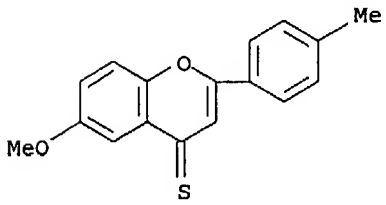
RN 16074-59-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 82340-44-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

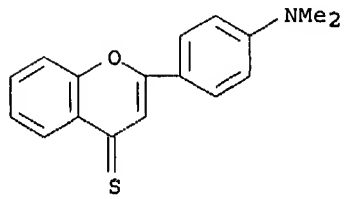


RN 223594-07-8 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-methoxy-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 13 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:583952 HCAPLUS
DOCUMENT NUMBER: 129:267530
TITLE: Vectorial and octupolar components of the first-order hyperpolarizability in push-pull benzopyranic series
AUTHOR(S): Illien, Bertrand; Botrel, Alain
CORPORATE SOURCE: Laboratoire de Physicochimie, Ecole Nationale Superieure de Chimie, Rennes, F-35700, Fr.
SOURCE: Molecular Engineering (1998), 8(1), 1-7
CODEN: MOLEEV; ISSN: 0925-5125
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Vectorial (weight 1) and octupolar (weight 3) components of the 1st-order hyperpolarizability are computed using the PM3/RHF/FF method following 2 different decomposition schemes. These calcns. evidence the importance of the weight 3 component of the P tensor even in push-pull mols. The 3 values, output from the 2 decomposition schemes, are different but show the same evolutionary trend within benzopyranic mol. series. The square root of a macroscopic square average quantity <β2>1/2 (which is usually determined in elastic 2nd-harmonic light scattering experiment) is then computed and compared to the norm of the mol. β Cartesian tensor.
IT **210550-35-9**
RL: PRP (Properties)
(vectorial and octupolar components of first-order hyperpolarizability in)
RN 210550-35-9 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-[4-(dimethylamino)phenyl]- (9CI) (CA INDEX NAME)

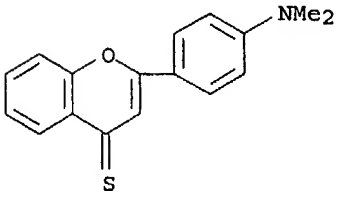


REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 14 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:428156 HCAPLUS
DOCUMENT NUMBER: 129:142320
TITLE: Synthesis and theoretical and experimental nonlinear optical studies of push-pull benzopyranic derivatives containing an oxo, thioxo or dicyanoethylene group as acceptor site
AUTHOR(S): Illien, Bertrand; Jehan, Philippe; Botrel, Alain; Darchen, Andre; Ledoux, Isabelle; Zyss, Joseph; Le Magueres, Pierre; Ouahab, Lahcene
CORPORATE SOURCE: Laboratoire de Physicochimie, Ec. Natl. Super. Chim., Rennes, 35700, Fr.
SOURCE: New Journal of Chemistry (1998), 22(6), 633-641
CODEN: NJCHE5; ISSN: 1144-0546
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of new push-pull mols., containing 4H-1-benzopyran-4-oxo-2-yl, 4H-1-benzopyran-4-thioxo-2-yl or 4H-1-benzopyran-4-(ylidene malononitrile)-2-yl as acceptor site and 4-dimethylaminophenyl or ferrocenyl as donor site, was synthesized and characterized. The X-ray structures of 2-(4'-dimethylaminophenyl)-4H-1-benzopyran-4-thione and 2-(4'-dimethylaminophenylethenyl)-4H-1-benzopyran-4-thione were established. Exptl. dipole moments and first-order hyperpolarizability β data measured in solution by elec.-field-induced second-harmonic generation (EFISHG) were compared to computed values obtained by the semiempirical PM3 method for optimized structures. The characteristics of the lowest energy singlet-singlet π π* transitions were determined through UV/VIS spectral measurements and semiempirical CNDO/S-CIS calcns. All of the exptl. and computed results point out the NLO efficiency of the acceptor thioxo group, which was compared to the well-known aldehyde or dicyanomethylene substituents.

IT **210550-35-9P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and theor. and exptl. nonlinear optical studies of push-pull benzopyranic derivs. containing oxo, thioxo or dicyanoethylene group as acceptor site)
RN 210550-35-9 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-[4-(dimethylamino)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 94 THERE ARE 94 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

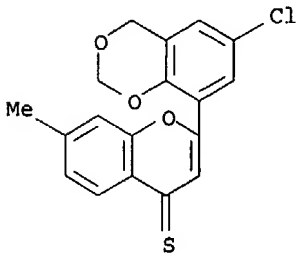
L32 ANSWER 15 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:61146 HCAPLUS
DOCUMENT NUMBER: 128:167299
TITLE: Synthetic analogs of natural flavolignans VIII. Synthesis of 6-chloro-1,3-benzodioxane, 1,4-benzodioxane, 1,5-benzodioxepane, and 1,6-benzodioxocane analogs of 4-thioflavone
AUTHOR(S): Aitmambetov, A.; Berdimbetova, G.; Khilya, V. P.
CORPORATE SOURCE: KIEN, Karakalpak Division, Academy of Sciences of the Republic of Uzbekistan, Uzbekistan
SOURCE: Chemistry of Natural Compounds (Translation of Khimiya Prirodnykh Soedinenii) (1997), 33(3), 286-288
CODEN: CHNCA8; ISSN: 0009-3130
PUBLISHER: Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English

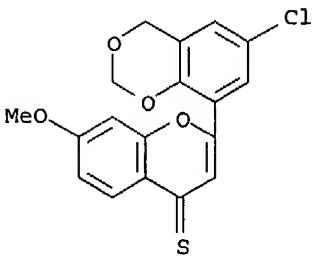
AB 1,3-Benzodioxane, 1,4-benzodioxane, 1,5-benzodioxepane, and 1,6-benzodioxocane analogs of 4-thioflavone, e.g. I, were synthesized from the flavonoid by reaction with P2S5.

IT **147723-18-0P 147723-19-1P 147723-20-4P 147723-21-5P 147723-22-6P 202914-90-7P 202914-91-8P 202914-92-9P 202914-93-0P 202914-94-1P 202914-95-2P 202914-96-3P 202914-97-4P 202914-98-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 6-chloro-1,3-benzodioxane, 1,4-benzodioxane, 1,5-benzodioxepane, and 1,6-benzodioxocane analogs of 4-thioflavone)

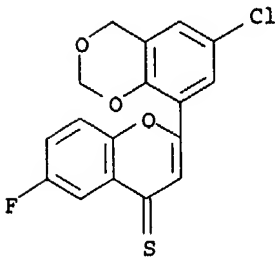
RN 147723-18-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(6-chloro-4H-1,3-benzodioxin-8-yl)-7-methyl- (9CI) (CA INDEX NAME)



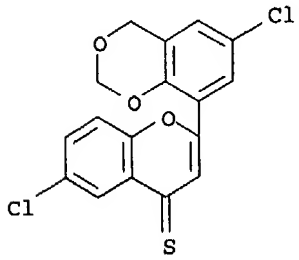
RN 147723-19-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(6-chloro-4H-1,3-benzodioxin-8-yl)-7-methoxy- (9CI) (CA INDEX NAME)



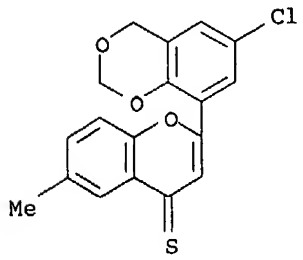
RN 147723-20-4 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(6-chloro-4H-1,3-benzodioxin-8-yl)-6-fluoro- (9CI) (CA INDEX NAME)



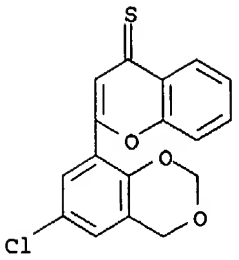
RN 147723-21-5 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-chloro-2-(6-chloro-4H-1,3-benzodioxin-8-yl)- (9CI) (CA INDEX NAME)



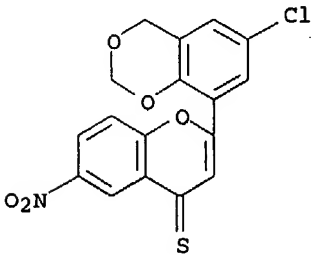
RN 147723-22-6 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(6-chloro-4H-1,3-benzodioxin-8-yl)-6-methyl- (9CI) (CA INDEX NAME)



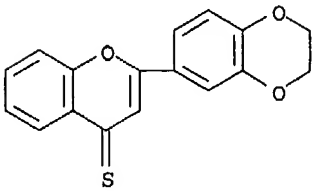
RN 202914-90-7 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(6-chloro-4H-1,3-benzodioxin-8-yl)- (9CI) (CA INDEX NAME)



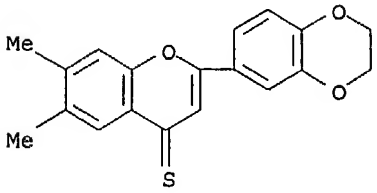
RN 202914-91-8 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(6-chloro-4H-1,3-benzodioxin-8-yl)-6-nitro- (9CI) (CA INDEX NAME)



RN 202914-92-9 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(2,3-dihydro-1,4-benzodioxin-6-yl)- (9CI) (CA INDEX NAME)

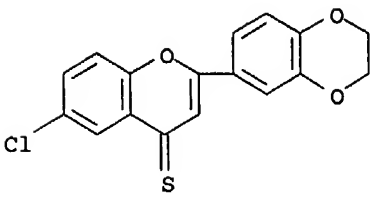


RN 202914-93-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(2,3-dihydro-1,4-benzodioxin-6-yl)-6,7-dimethyl- (9CI) (CA INDEX NAME)

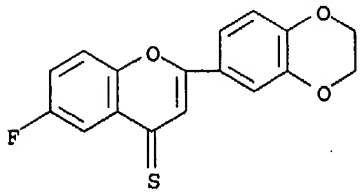


RN 202914-94-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-chloro-2-(2,3-dihydro-1,4-benzodioxin-6-yl)-

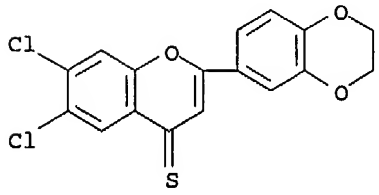
(9CI) (CA INDEX NAME)



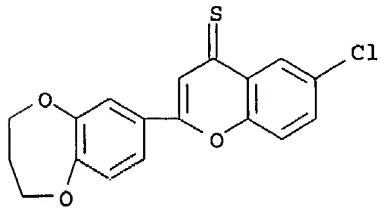
RN 202914-95-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(2,3-dihydro-1,4-benzodioxin-6-yl)-6-fluoro-
(9CI) (CA INDEX NAME)



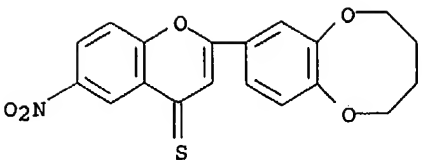
RN 202914-96-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6,7-dichloro-2-(2,3-dihydro-1,4-benzodioxin-6-
yl)- (9CI) (CA INDEX NAME)



RN 202914-97-4 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-chloro-2-(3,4-dihydro-2H-1,5-benzodioxepin-7-
yl)- (9CI) (CA INDEX NAME)



RN 202914-98-5 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-nitro-2-(2,3,4,5-tetrahydro-1,6-benzodioxocin-
8-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 16 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:169157 HCAPLUS
DOCUMENT NUMBER: 126:225315
TITLE: Bicyclic heterocyclic derivatives having α1-adrenergic and 5HT1A serotonergic activities
INVENTOR(S): Leonardi, Amedeo; Motta, Gianni; Riva, Carlo; Testa, Rodolfo
PATENT ASSIGNEE(S): Recordati S.A., Chemical and Pharmaceutical Company, Switz.
SOURCE: U.S., 84 pp., Cont.-in-part of U.S. 5,474,994.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

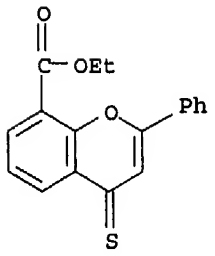
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5605896	A	19970225	US 1994-299188	19940831
US 5403842	A	19950404	US 1992-888775	19920526
AU 9336296	A1	19930913	AU 1993-36296	19930223
RO 112111	B3	19970530	RO 1994-1404	19930223
PL 175556	B1	19990129	PL 1993-304889	19930223
RU 2128656	C1	19990410	RU 1994-43324	19930223
SK 280143	B6	19990910	SK 1994-1007	19930223
ZA 9301278	A	19931118	ZA 1993-1278	19930224
LT 3038	B	19940925	LT 1993-354	19930224
CN 1079738	A	19931222	CN 1993-105852	19930526
CN 1040434	B	19981028		
US 5474994	A	19951212	US 1993-67861	19930526
FI 9403876	A	19940823	FI 1994-3876	19940823
NO 9403140	A	19940825	NO 1994-3140	19940825
PRIORITY APPLN. INFO.:			IT 1992-MI408 A	19920225
			US 1992-888775 A2	19920526
			US 1993-67861 A2	19930526
			EP 1993-301264 A	19930222
			WO 1993-EP420 A	19930223

OTHER SOURCE(S): MARPAT 126:225315
AB Bicyclic heterocyclic derivs., such as I [X = N, O, S; W = C(O), C(S), CH(OH), bond; R2 = H, optionally substituted alkyl, alkenyl, alkylnyl, carbocycle, heterocycle; R3 = alkyl, hydroxyalkyl, Ph, OH, alkoxy, alkoxyalkyl; R6 = H, halogen, NO2, NH2, AcNH, mono-, dialkylamino, CN, OH, alkoxy, alkyl; Y = CO, CO2, CONH, CH(OH), CH:CH, CH:CHCO2, CH:CHCONH, CH2NH, CH2NHCO, CH2NHSO2, CH2O, CH2S, NH, NHCO, NHCONH, NHSO2, O, S, SO2NH, CONHO, CSNH, NHCO2, COS, CONH(CH2)m, m = 1-6; Z = N, A = (un)substituted Ph, pyrimidinyl, 1,4-benzodioxan-8-yl, benzopyran-8-yl, benzofuran-7-yl, dihydrobenzopyran-8-yl; Z = CH2N; Z = CH, A = one or two

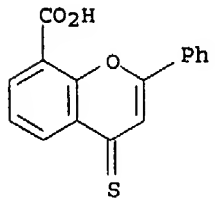
Ph, 4-FC6H4CO, 2-oxo-1-benzimidazolinyl, (CH2)nOA, n = 0-2], and their pharmaceutically acceptable salts useful as α1-adrenergic and 5HT1A serotonergic agents for the treatment of hypertension, urethral and lower urinary tract contractions, and other disorders are described. Thus, benzopyran II was prepared by heating 1-(2-methoxyphenyl)piperazine with benzopyran III at 180° for 5 h. II had IC50 = 29 nM for α1-adrenergic receptor binding, IC50 = 9 nM for 5HT1A receptor binding, ED25 = 45 μg/kg i.v. hypotensive effect and ED25 = 1.4 μg/kg in Na-induced urethral contractility assays.

IT **174765-50-5P 174765-51-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bicyclic heterocyclic derivs. having α1-adrenergic and 5HT1A serotonergic activities)

RN 174765-50-5 HCAPLUS
CN 4H-1-Benzopyran-8-carboxylic acid, 2-phenyl-4-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 174765-51-6 HCAPLUS
CN 4H-1-Benzopyran-8-carboxylic acid, 2-phenyl-4-thioxo- (9CI) (CA INDEX NAME)



L32 ANSWER 17 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:41112 HCAPLUS
DOCUMENT NUMBER: 126:164144
TITLE: The photophysics of thioflavone in solution
AUTHOR(S): Maciejewski, A.; Szymanski, M.; Steer, R. P.
CORPORATE SOURCE: Faculty of Chemistry, A. Mickiewicz University, Poznan, Pol.
SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (1996), 100(1-3), 43-52
CODEN: JPPCEJ; ISSN: 1010-6030
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal

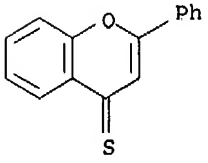
LANGUAGE: English

AB The absorption, emission and emission excitation spectra, S2→S0 fluorescence and T1→S0 phosphorescence quantum yields and S2 and T1 excited state lifetimes of thioflavone (TF) were measured in perfluoro-1,3-dimethylcyclohexane (PFDMCH) and 3-methylpentane (3-MP) at room temperature The results were analyzed to provide a quant. description of the decay processes of excited TF, with emphasis on the effect of the Ph rotor on the radiationless decay rates. In the inert perfluoroalkane solvent, both S2 and T1 relax intramolecularly via an S2→S1→T1→S0 path. S2→S0 fluorescence and T1→S0 phosphorescence also account for a small fraction of the excited state decay events, but no thermally activated delayed fluorescence, S1→S0+hvdf, is observed In 3-MP, the decay mechanism is dominated by intermol. interactions between excited TF and the solvent. The rates of intramol. radiationless decay are larger in TF than in rigid thiones having the same electronic energy gaps owing to the influence of the torsional motion of the Ph group. By comparison of the observed rate consts. for intramol. radiationless decay of excited TF with those of a hypothetical rigid thione having the same electronic energy spacings, contributions to the radiationless decay rates of S2 and T1 due to torsional motion of the Ph group were quantified. The second-order rate consts. for quenching of triplet thione by mol. oxygen and by ground state thione were also measured. Excitation of TF to singlet excited states higher in energy than S2 results in decay to S1 and T1 which partially bypasses S2.

IT **5465-04-3**, 2-Phenyl-chromene-4-thione
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(photophysics of thioflavone in solution)

RN 5465-04-3 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 18 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:288893 HCAPLUS

DOCUMENT NUMBER: 125:10413

TITLE: Synthesis and biological evaluation of flavonoids and related compounds as gastroprotective agents

AUTHOR(S): Ares, Jeffrey J.; Outt, Pamela E.; Randall, Jared L.; Johnston, Jeffrey N.; Murray, Peter D.; O'Brien, Linda M.; Weisshaar, Pamela S.; Ems, Beth L.

CORPORATE SOURCE: Miami Valley Labs., Procter & Gamble Company, Cincinnati, OH, 45253-8707, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(8), 995-998
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

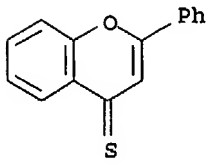
LANGUAGE: English

AB Several analogs I (R = 2-thienyl, 3-pyridyl, and 1-methyl-2-indolyl) of the gastroprotective mol. flavone were synthesized and evaluated for gastroprotective activity. A C2-C3 double bond and an intact C ring appear necessary for optimum activity. Activity can be retained by replacing the 2-Ph substituent with other groups but is eliminated when this ring is moved from the 2- to the 3-position.

IT **5465-04-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis and biol. evaluation of flavonoids and related compds. as gastroprotective agents)

RN 5465-04-3 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 19 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:35000 HCAPLUS

DOCUMENT NUMBER: 124:232248

TITLE: Benzopyran derivatives having affinity for α1-adrenergic and 5HT1A-serotoninergic receptors

INVENTOR(S): Leonardi, Amedeo; Motta, Gianni; Riva, Carlo; Testa, Rodolfo

PATENT ASSIGNEE(S): Recordati S.A., Chemical and Pharmaceutical Company, Switz.

SOURCE: U.S., 37 pp. Cont.-in-part of U.S. 5,403,842.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5474994	A	19951212	US 1993-67861	19930526
US 5403842	A	19950404	US 1992-888775	19920526
EP 558245	A1	19930901	EP 1993-301264	19930222
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
AU 9336296	A1	19930913	AU 1993-36296	19930223
RO 112111	B3	19970530	RO 1994-1404	19930223
PL 175556	B1	19990129	PL 1993-304889	19930223
SK 280143	B6	19990910	SK 1994-1007	19930223
CN 1079738	A	19931222	CN 1993-105852	19930526
CN 1040434	B	19981028		
FI 9403876	A	19940823	FI 1994-3876	19940823
NO 9403140	A	19940825	NO 1994-3140	19940825
US 5605896	A	19970225	US 1994-299188	19940831
PRIORITY APPLN. INFO.:			US 1992-888775 A2	19920526
			EP 1993-301264 A	19930222
			IT 1992-MI408 A	19920225

WO 1993-EP420 A 19930223
US 1993-67861 A2 19930526

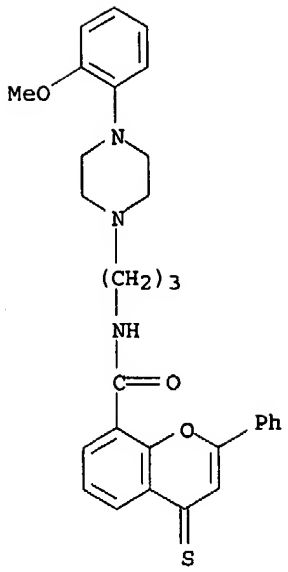
OTHER SOURCE(S): MARPAT 124:232248

AB This invention provides bicyclic heterocyclic derivs. I wherein the dotted line represents a single or double bond; X represents a nitrogen, oxygen or sulfur atom, or an amino or alkylamino group, a sulfinyl or sulfonyl group; W represents a carbonyl, thiocarbonyl, hydroxymethylene, or a methylene group or a bond; or when X is nitrogen and W is a methine, the fused rings represent a quinoline; R2 represents, e.g, a hydrogen atom or an alkyl, alkenyl, alkynyl, carbocyclic or heterocyclic group, each of which groups may optionally be substituted; or R2 itself represents a trifluoromethyl or an aroyl group; R3 represents a hydrogen atom or an alkyl, hydroxyalkyl, alkyl-O-R4 Ph, hydroxy, or O-R4, wherein R4 represents an alkyl group optionally substituted with an aryl group; R6 represents a hydrogen or halogen atom or a nitro, amino, acylamino, alkylsulfonylamino, alkylamino, dialkylamino, cyano, hydroxy, alkoxy or alkyl group; R7 represents a hydrogen atom or an alkoxy group; Y = e.g., CO, COO, CONH; Z represents a linear or branched chain alkylene group having from 1 to 6 carbon atoms and optionally having one hydroxy substituent; B = e.g., II, n = 1 or 2, A = substituted Ph, 2-pyrimidinyl; and their pharmaceutically acceptable salts useful for the treatment of hypertension, urethral and lower urinary tract contractions, and other disorders. The compds. are also useful for binding α1-adrenergic and 5HT1A serotonergic receptors, in vitro or in vivo. Thus, e.g., esterification of 8-carboxy-3-methyl-4-oxo-2-phenyl-4H-1-benzopyran with 1-(3-chloropropyl)-4-(2-methoxyphenyl)piperazine followed by HCl treatment afforded 8-{3-[4-(2-methoxyphenyl)-1-piperazinyl]propoxycarbonyl}-3-methyl-4-oxo-2-phenyl-4H-1-benzopyran dihydrochloride (III.2HCl) which exhibited IC50's of 20 and 19 nM, resp., for α1 and 5-HT1A receptor binding. Data were also presented for the effect of I on K+ stimulation of rat bladder strips, and on urethral contractions and blood pressure in dogs.

IT **174765-20-9P 174765-21-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(benzopyran derivs. having affinity for α1-adrenergic and 5HT1A-serotoninergic receptors)

RN 174765-20-9 HCAPLUS

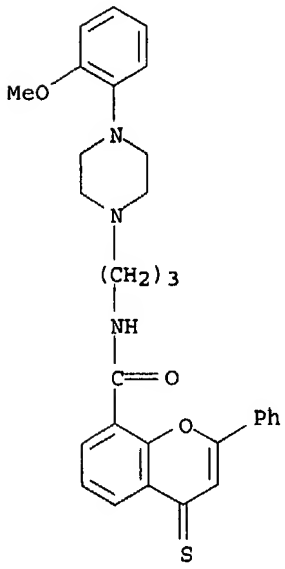
CN 4H-1-Benzopyran-8-carboxamide, N-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-2-phenyl-4-thioxo- (9CI) (CA INDEX NAME)



RN 174765-21-0 HCAPLUS
CN 4H-1-Benzopyran-8-carboxamide, N-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-2-phenyl-4-thioxo-, monomethanesulfonate (9CI) (CA INDEX NAME)

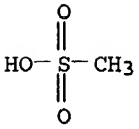
CM 1

CRN 174765-20-9
CMF C30 H31 N3 O3 S

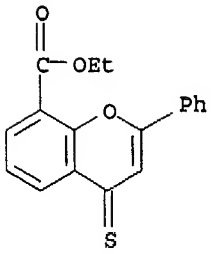


CM 2

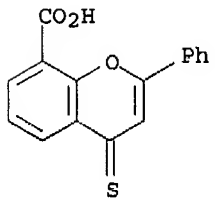
CRN 75-75-2
CMF C H4 O3 S



IT **174765-50-5P 174765-51-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(benzopyran derivs. having affinity for α1-adrenergic and 5HT1A-serotoninergic receptors)
RN 174765-50-5 HCAPLUS
CN 4H-1-Benzopyran-8-carboxylic acid, 2-phenyl-4-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 174765-51-6 HCAPLUS
CN 4H-1-Benzopyran-8-carboxylic acid, 2-phenyl-4-thioxo- (9CI) (CA INDEX NAME)

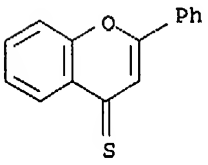


L32 ANSWER 20 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:634201 HCAPLUS
DOCUMENT NUMBER: 124:3032
TITLE: Evaluation of a broad variety of coumarins, chromones, their furohomologues and thione analogs as phototoxins activated by UVA and visible light
AUTHOR(S): Borges, Marta L.; Matos, Olivia C.; Pais, Isabel; de

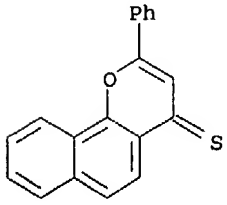
Melo, J. Seixas; Ricardo, Candido P.; Macanita, Antonio; Becker, Ralph S.
CORPORATE SOURCE: Inst. Tecnol. Quim. Biol., Rua da Quinta Grande, Oeiras, P-2780, Port.
SOURCE: Pesticide Science (1995), 44(2), 155-62
CODEN: PSSCBG; ISSN: 0031-613X
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The potential of a new kind of light-induced pesticide action was evaluated for a broad variety (32) of natural photosensitizers and their thione derivs. The latter were synthesized to shift the absorption spectra towards the visible region and to increase the triplet and singlet oxygen quantum yields. Qual. and quant. evaluation of growth inhibition of Fusarium culmorum (F. G. Smith) Sacc. produced by these photosensitizers under UVA and visible light was performed on silica gel plates and in liquid medium. The results show that the phototoxicity per excited mol. of the thione derivs. using UVA light was similar to that of their parent natural compds. On the other hand, only the thione derivs. were photoactive under visible light irradiation These compds. show encouraging levels of phototoxicity against F. culmorum, both in liquid culture and on silica plates, and may have potential for use as photoactive pesticides.

IT **5465-04-3 14882-98-5 171119-01-0**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(phototoxicity of)

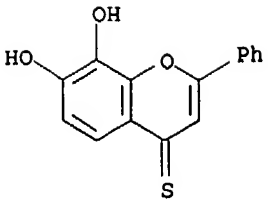
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



RN 14882-98-5 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-phenyl- (8CI, 9CI) (CA INDEX NAME)



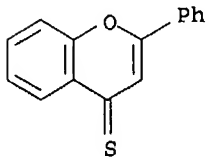
RN 171119-01-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7,8-dihydroxy-2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 21 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:457316 HCAPLUS
DOCUMENT NUMBER: 121:57316
TITLE: Photochemical reactions of bianthrone and related substances
AUTHOR(S): Abdou, Wafaa M.; Elkhoshnieh, Yehia O.; Sidky, Mahmoud M.
CORPORATE SOURCE: Natl. Res. Cent., Cairo, Egypt
SOURCE: Tetrahedron (1994), 50(11), 3595-602
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Photocleavage reactions of a wide range of ethylene compds. I (X = CO, O, S. NMe, etc.) were studied. Photosensitized oxygenation gave their corresponding ketones. However, photoreaction of these substrates with elemental S yielded the corresponding thioketones. Also, photochem. behavior of some ethylene episulfides also was studied. It could be concluded that UV-irradiation provides a rapid and effective deactivation pathway for this class of compds.

IT **5465-04-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in photochem. reaction of bianthrone)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 22 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:457275 HCAPLUS
DOCUMENT NUMBER: 121:57275
TITLE: Synthesis and hypolipidemic activity of novel 4-oxo- and 4-thioxo-4H benzopyran-2-phenylalkanoic acids and esters
AUTHOR(S): Orjales, A.; Berisa, A.; Alonso-Cires, L.
CORPORATE SOURCE: Dep. Invest., FAES, SA, Leioa, Spain
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1994), 33B(1), 27-31
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal

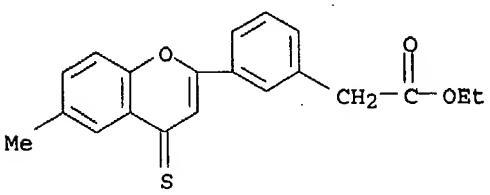
LANGUAGE: English

AB Novel title compds. I (X = O, S, R = 3- or 4-CHR3CO2R2; R1 = H, 6-Me, 5,7-Me2; R3 = H, Me, R4 = H, Me, Et, Pr, CHMe2, Bu, CH2CHMe2, octyl, cetyl) were prepared and evaluated for their hypolipidemic activity. Among these compds. 3'-alkanoyl derivs. show superior activity, decreasing total cholesterol, triglycerides and phospholipids in the serum of mice treated with Triton WR 1339. Introduction of a Me group in the 4-oxo-4H-benzopyran system greatly decreases the activity. Propionic acid derivs. are less active than the acetic acid derivs. On the other hand, Me substitution in the 4-thioxo compds. leads to an increase in activity. I (R = 3-CH2CO2Et, 3-CH2CO2Me; R1 = H, X = O; R1 = 6-Me, X = S) are the most active compds.

IT **155938-48-0P 155938-58-2P 155938-59-3P 155938-64-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and hypolipidemic activity of)

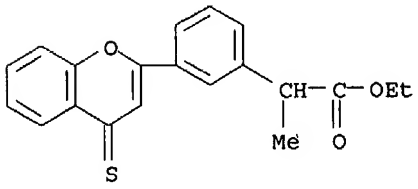
RN 155938-48-0 HCAPLUS

CN Benzeneacetic acid, 3-(6-methyl-4-thioxo-4H-1-benzopyran-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)



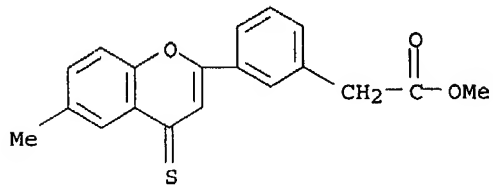
RN 155938-58-2 HCAPLUS

CN Benzeneacetic acid, α-methyl-3-(4-thioxo-4H-1-benzopyran-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

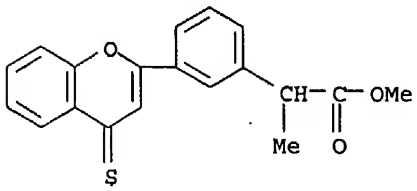


RN 155938-59-3 HCAPLUS

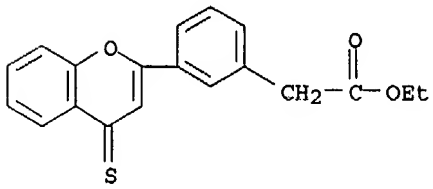
CN Benzeneacetic acid, 3-(6-methyl-4-thioxo-4H-1-benzopyran-2-yl)-, methyl ester (9CI) (CA INDEX NAME)



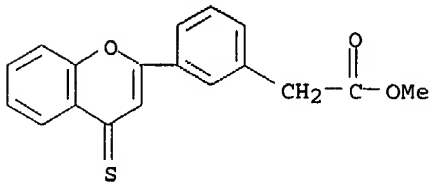
RN 155938-64-0 HCAPLUS
CN Benzeneacetic acid, α-methyl-3-(4-thioxo-4H-1-benzopyran-2-yl)-, methyl ester (9CI) (CA INDEX NAME)



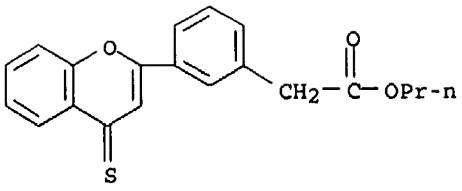
IT **155938-47-9P 155938-49-1P 155938-50-4P**
155938-51-5P 155938-52-6P 155938-53-7P
155938-54-8P 155938-55-9P 155938-56-0P
155938-57-1P 155938-60-6P 155938-61-7P
155938-62-8P 155938-63-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 155938-47-9 HCAPLUS
CN Benzeneacetic acid, 3-(4-thioxo-4H-1-benzopyran-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)



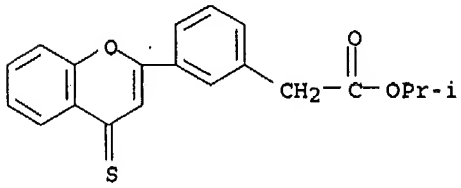
RN 155938-49-1 HCAPLUS
CN Benzeneacetic acid, 3-(4-thioxo-4H-1-benzopyran-2-yl)-, methyl ester (9CI) (CA INDEX NAME)



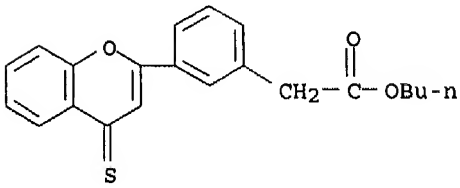
RN 155938-50-4 HCAPLUS
CN Benzeneacetic acid, 3-(4-thioxo-4H-1-benzopyran-2-yl)-, propyl ester (9CI) (CA INDEX NAME)



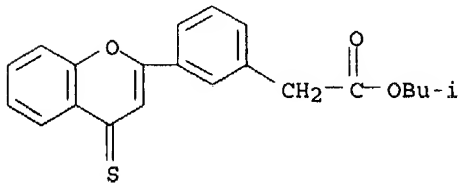
RN 155938-51-5 HCAPLUS
CN Benzeneacetic acid, 3-(4-thioxo-4H-1-benzopyran-2-yl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)



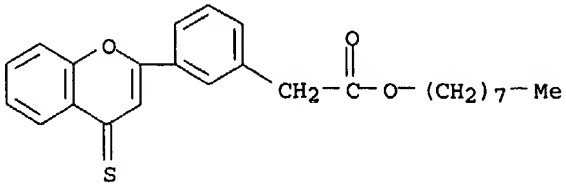
RN 155938-52-6 HCAPLUS
CN Benzeneacetic acid, 3-(4-thioxo-4H-1-benzopyran-2-yl)-, butyl ester (9CI) (CA INDEX NAME)



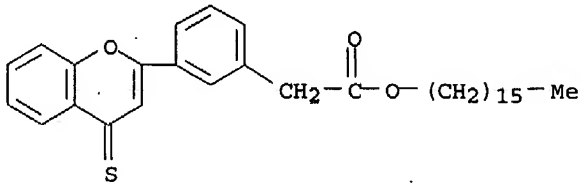
RN 155938-53-7 HCAPLUS
CN Benzeneacetic acid, 3-(4-thioxo-4H-1-benzopyran-2-yl)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



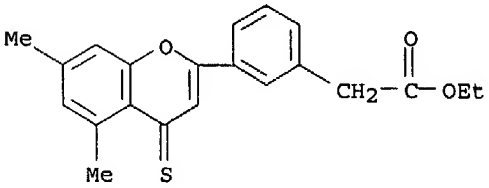
RN 155938-54-8 HCAPLUS
CN Benzeneacetic acid, 3-(4-thioxo-4H-1-benzopyran-2-yl)-, octyl ester (9CI) (CA INDEX NAME)



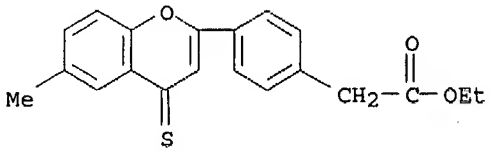
RN 155938-55-9 HCAPLUS
CN Benzeneacetic acid, 3-(4-thioxo-4H-1-benzopyran-2-yl)-, hexadecyl ester (9CI) (CA INDEX NAME)



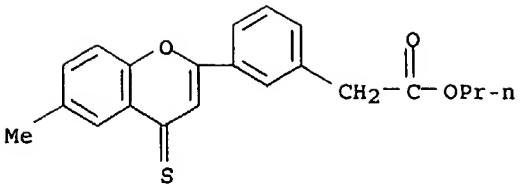
RN 155938-56-0 HCAPLUS
CN Benzeneacetic acid, 3-(5,7-dimethyl-4-thioxo-4H-1-benzopyran-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)



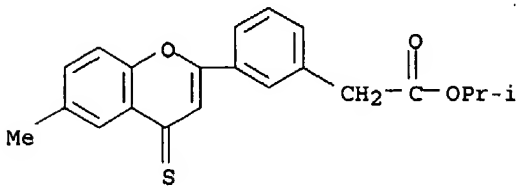
RN 155938-57-1 HCAPLUS
CN Benzeneacetic acid, 4-(6-methyl-4-thioxo-4H-1-benzopyran-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)



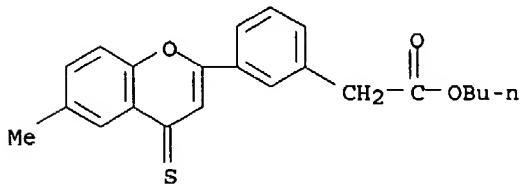
RN 155938-60-6 HCAPLUS
CN Benzeneacetic acid, 3-(6-methyl-4-thioxo-4H-1-benzopyran-2-yl)-, propyl ester (9CI) (CA INDEX NAME)



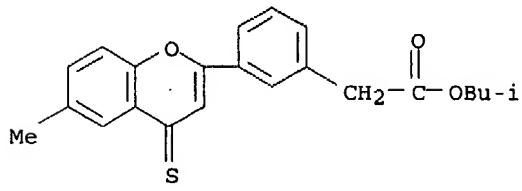
RN 155938-61-7 HCAPLUS
CN Benzeneacetic acid, 3-(6-methyl-4-thioxo-4H-1-benzopyran-2-yl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 155938-62-8 HCAPLUS
CN Benzeneacetic acid, 3-(6-methyl-4-thioxo-4H-1-benzopyran-2-yl)-, butyl ester (9CI) (CA INDEX NAME)

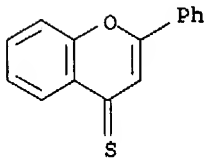


RN 155938-63-9 HCAPLUS
CN Benzeneacetic acid, 3-(6-methyl-4-thioxo-4H-1-benzopyran-2-yl)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

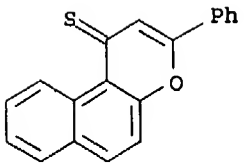


L32 ANSWER 23 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:179861 HCAPLUS
DOCUMENT NUMBER: 120:179861
TITLE: Photoelectron (HeI) spectroscopy of flavonoids and thioflavanoids. II. Photoelectron spectra of chromone and 1-thiochromone derivatives
AUTHOR(S): Dinya, Zoltan; Sztaricskai, Ferenc

CORPORATE SOURCE: Res. Group Antibiot., Hung. Acad. Sci., Debrecen, H-4010, Hung.
SOURCE: Croatica Chemica Acta (1993), 66(2), 265-78
CODEN: CCACAA; ISSN: 0011-1643
DOCUMENT TYPE: Journal
LANGUAGE: English
AB HeI photoelectron spectra of some chromanone and chromone derivs. (flavanone, isoflavanone, flavone and isoflavone), their thio analogs, and sulfoxide and sulfone derivs., resp., were measured in the gas phase and the data evaluated by means of semiempirical MO evaluations (HAM/3 and CNDO/S) and by the PMO theory.
IT **5465-04-3**
RL: PRP (Properties)
(photoelectron gas phase spectra of, semiempirical MO evaluations for)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 24 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:77163 HCAPLUS
DOCUMENT NUMBER: 120:77163
TITLE: Self-assembling chiral metallo-clefts; synthesis and molecular structure of N,N'-bis(12H-benzo[a]xanthen-12-ylidene)-1,2-ethanediamine zinc(II) dichloride complex
AUTHOR(S): Barf, Tjeerd; Jansen, Johan F. G. A.; van Bolhuis, Fre; Spek, Anthony L.; Feringa, Ben L.
CORPORATE SOURCE: Groningen Cent. Catal. Synth., Univ. Groningen, Groningen, 9747 AG, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1993), 112(6), 376-83
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:77163
AB Bulky ligands for cleft-type metal complexes were prepared from thio ketones and diamines in yields varying from 20-80%. A mol. structure determination of one ligand N,N'-bis(benzoxanthenylidene)propanediamine I was performed. A metallocleft was constructed by a self-assembling process with ZnCl2. A crystallog. study of this I-Zn complex revealed surprisingly that an anti-syn inversion of the imine moieties of the ligand had taken place during complexation.
IT **139448-82-1P**, 3-Phenyl-1H-naphtho[2,1-b]pyran-1-thione
RL: SPN (Synthetic preparation); PREP (Preparation)
(intermediate in preparation of bis(benzo[a]xanthenylidene)propanediamine ligands)
RN 139448-82-1 HCAPLUS
CN 1H-Naphtho[2,1-b]pyran-1-thione, 3-phenyl- (9CI) (CA INDEX NAME)

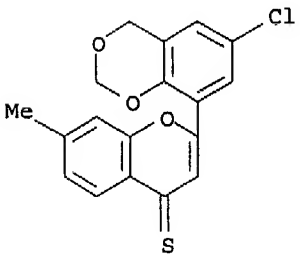


L32 ANSWER 25 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1993:254837 HCAPLUS
DOCUMENT NUMBER: 118:254837
TITLE: Chemistry of isoflavone heteroanalogs. 13. 1,3-Benzodioxan analogs of flavonoids
AUTHOR(S): Khilya, V. P.; Al Budy, H.; Aitmambetov, A.; Grishko, L. G.; Turov, A. V.; Zakharik, D. M.; Litkei, D.
CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, Ukraine
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1992), (7), 879-87
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian

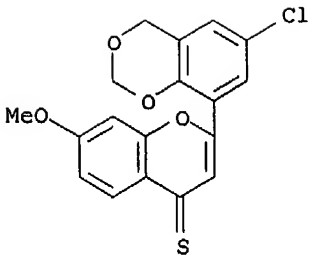
AB 1,3-Benzodioxan analogs of chalcones I (R1 = H, 4-, 5-Me, 4,5-Me2, 4-MeO, 5-halo, R2 = Cl, Br) and their epoxides were synthesized. A variety of pyrazolines, e.g. II (R = Ph, Me), novel flavones, e.g. III, and flavonoid analogs of the flavolignan silibinin were prepared NMR spectra were determined for the synthesized compds.

IT **147723-18-0P 147723-19-1P 147723-20-4P**
147723-21-5P 147723-22-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

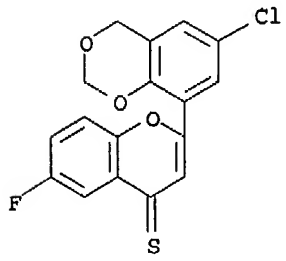
RN 147723-18-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(6-chloro-4H-1,3-benzodioxin-8-yl)-7-methyl- (9CI) (CA INDEX NAME)



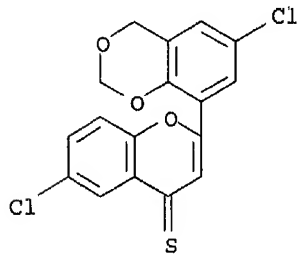
RN 147723-19-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(6-chloro-4H-1,3-benzodioxin-8-yl)-7-methoxy- (9CI) (CA INDEX NAME)



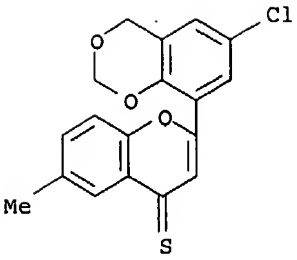
RN 147723-20-4 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(6-chloro-4H-1,3-benzodioxin-8-yl)-6-fluoro-
(9CI) (CA INDEX NAME)



RN 147723-21-5 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-chloro-2-(6-chloro-4H-1,3-benzodioxin-8-yl)-
(9CI) (CA INDEX NAME)



RN 147723-22-6 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(6-chloro-4H-1,3-benzodioxin-8-yl)-6-methyl-
(9CI) (CA INDEX NAME)

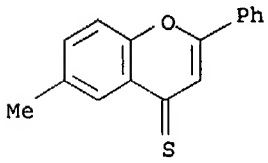


L32 ANSWER 26 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:214399 HCAPLUS
DOCUMENT NUMBER: 116:214399
TITLE: Benzo-γ-pyrones. Part XIV. Reaction of C-substituted 2-phenyl-4H-1-benzopyran-4-ones with hydroxylamine
AUTHOR(S): Basinski, Wlodzimierz
CORPORATE SOURCE: Fac. Pharm., Sch. Med., Lodz, 90151, Pol.
SOURCE: Polish Journal of Chemistry (1991), 65(9-10), 1619-32
CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English

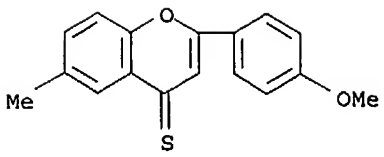
AB The reaction of flavones I (R, R1 = H, Me; R2 = H, Me, Br; R3 = H, MeO) with hydroxylamine in anhydrous pyridine was investigated. The oximes II and isoxazoles III were the products. It was determined that the ratio of II to III is dependent on the nature of substituent and its position in the flavone skeleton. It is postulated that the flavone is an ambient electrophile and that the reaction course is characteristic for this class of compds.

IT **140885-77-4P 140885-97-8P 140885-98-9P**
140885-99-0P 140886-00-6P 140886-01-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oximation of)

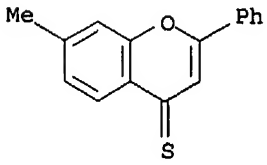
RN 140885-77-4 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



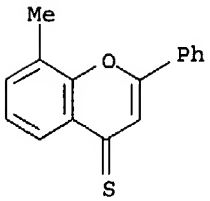
RN 140885-97-8 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)



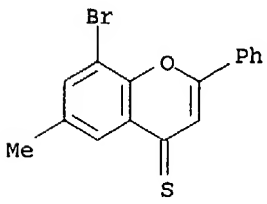
RN 140885-98-9 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7-methyl-2-phenyl- (9CI) (CA INDEX NAME)



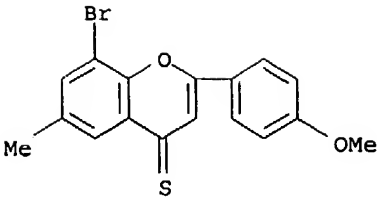
RN 140885-99-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 8-methyl-2-phenyl- (9CI) (CA INDEX NAME)



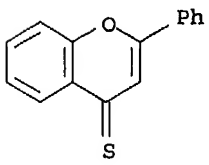
RN 140886-00-6 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 8-bromo-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



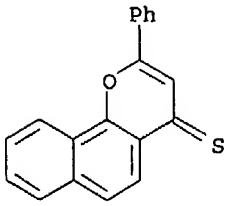
RN 140886-01-7 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 8-bromo-2-(4-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)



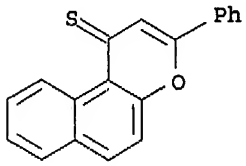
L32 ANSWER 27 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:128584 HCAPLUS
DOCUMENT NUMBER: 116:128584
TITLE: Organophosphorus compounds. Action of 2,4-bis(4-methoxyphenyl)-1,3,2,4-dithiaphosphetane 2,4-disulfide (Lawesson reagent) and 2,4-bis(phenylthio)-1,3-dithia-2,4-diphosphetane 2,4-disulfide (Japanese reagent) on flavone, α-naphthoflavone and β-naphthoflavone
AUTHOR(S): Hafez, Taghrid S.
CORPORATE SOURCE: Dep. Pestic. Chem., Natl. Res. Cent., Cairo, Egypt
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1991), 63(3-4), 249-53
CODEN: PSSLEC; ISSN: 1042-6507
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Japanese reagent converts 2-phenyl-5,6-benzo-γ-pyrone into 2-phenyl-5,6-benzopyrane-4-thione. Lawesson reagent converts 2-phenyl-7,8-benzo-1,4-chromone (3a) and 2-phenyl-5,6-benzo-1,4-chromone (4a) into their corresponding thioketones. Thiation of 3a and 4a with Lawesson reagent can be induced photochem. to give the thioketones. Thiation of 3a and 4a with Japanese reagent is accompanied with ring opening at the heterocyclic oxygen atom of the γ-pyrone ring.
IT **5465-04-3P 14882-98-5P 139448-82-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



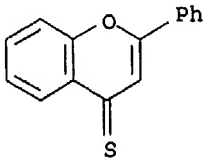
RN 14882-98-5 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-phenyl- (8CI, 9CI) (CA INDEX NAME)



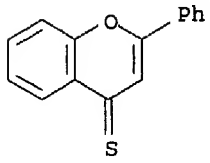
RN 139448-82-1 HCAPLUS
CN 1H-Naphtho[2,1-b]pyran-1-thione, 3-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 28 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:247084 HCAPLUS
DOCUMENT NUMBER: 114:247084
TITLE: Organophosphorus chemistry. 20. The behavior of certain γ-pyrone derivatives toward 2,4-bis(4-methoxyphenyl)-1,3,2,4-dithiaphosphetane-2,4-disulfide (Lawesson's reagent)
AUTHOR(S): Hafez, Taghrid S.; El-Khoshnieh, Yehia O.; Mahran, Mohamed R.; Atta, Sanaa M. S.
CORPORATE SOURCE: Dep. Pestic. Chem., Natl. Res. Cent., Dokki, Egypt
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1991), 56(1-4), 165-71
CODEN: PSSLEC; ISSN: 1042-6507
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:247084
AB Lawesson's reagent (I) converts 2,6-dimethyl-γ-pyrone (II) and flavone III (X = O) into their corresponding thio ketones in high yields. Thiation of flavone III (X = O) with I can be induced photochem. to give thioflavone III (X = S) together with a ring phosphorane product. Thiation of khellin IV (X = O) by I to give IV (X = S) is accompanied by demethylation of IV (X = S) to give desmethylthiokhellin. The behavior of γ-pyrones II, III (X = O) and IV (X = O) toward thiation with I was discussed in the light of the principle of vinylogy.
IT **5465-04-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)

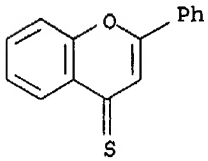


L32 ANSWER 29 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:86765 HCAPLUS
DOCUMENT NUMBER: 112:86765
TITLE: The cathodic coupling of heterocyclic activated thioketones. A new and efficient route to π-donors. (I)-The synthesis of polysubstituted bipyranylidenes from 4H-pyran-4-thiones
AUTHOR(S): Mabon, Gilles; Cariou, Michel; Simonet, Jacques
CORPORATE SOURCE: Lab. Electrochim., Univ. Cathol. Ouest, Angers, 49005, Fr.
SOURCE: New Journal of Chemistry (1989), 13(8-9), 601-7
CODEN: NJCHE5; ISSN: 0398-9836
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Activated 4H pyran-4-thiones may be coupled when reduced electrochem. in the presence of various electrophiles. Generally the reaction goes beyond the α dithiol or the α dithioether formation since an oxidative process (possibly of an electrocatalytic nature) may take place and leads via elimination to strongly donating compds. A new synthesis is described for various tetrasubstituted bipyranylidenes.
IT **5465-04-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, electrochem., on mercury and platinum, coupling in, Et bromide effect on)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)

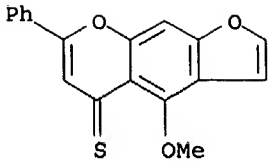


L32 ANSWER 30 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:454928 HCAPLUS
DOCUMENT NUMBER: 109:54928
TITLE: Cyclopalladated complexes of aromatic and heteroaromatic ligands containing unsaturated nitrogen or sulfur as donor atoms
AUTHOR(S): Davis, Robert C.; Grinter, Trevor J.; Leaver, Derek; O'Neil, Robert; Thomson, Gordon A.
CORPORATE SOURCE: Dep. Chem., Univ. Edinburgh, Edinburgh, EH9 3JJ, UK
SOURCE: Journal of Chemical Research, Synopses (1987), (9), 280-1
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal

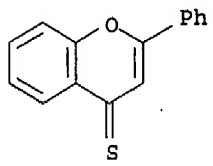
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:54928
AB Cyclopalladation of the title ligands by Na2PdCl4 or Li2PdCl4 in MeOH or MeOH/CH2Cl2 gave dimeric cyclopalladated complexes. E.g., treating xanthinethione with Na2PdCl4 in MeOH gave 90% cyclopalladated complex I. Similar results were obtained with Pd(OAc)2 in AcOH. Treating the dimeric chloro or acetoxy cyclopalladated complexes with NaS2CNR2/DMF or Et4NS2CNR2/CH2Cl2 (R = Me, Me2CH in both cases), resp., gave monomeric dithiocarbamato complexes. Thus, treating I with NaS2CNMe2/DMF gave 52% monomeric complex II. Also prepared were phosphine complexes, e.g., E- and Z-III.
IT **5465-04-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclopalladation of)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



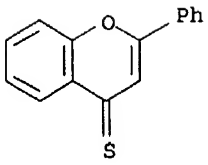
L32 ANSWER 31 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:84231 HCAPLUS
DOCUMENT NUMBER: 106:84231
TITLE: Synthesis of some visnagin derivatives with expected biological activity
AUTHOR(S): El-Sharief, A. M. S.; Ammar, M. S.; Mohamed, Y. A.
CORPORATE SOURCE: Fac. Sci., Al-Azhar Univ., Cairo, Egypt
SOURCE: Egyptian Journal of Chemistry (1985), Volume Date 1984, 27(4), 535-46
CODEN: EGJCA3; ISSN: 0367-0422
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Several visnagin derivs. I (R = Me, Et; R1 = H, 4-Me, 4-Cl, 2-Cl, 2-OMe) were prepared by condensation of R1CHO with the visnagin analog. I were treated with maleic anhydride to give cycloaddn. products. Aldehyde II and ester III were condensed with amines to yield imine and amide analogs. The resultant compds. were tested for fungicidal and bactericidal activity (no data).
IT **106751-65-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and biol. activity of)
RN 106751-65-9 HCAPLUS
CN 5H-Furo[3,2-g][1]benzopyran-5-thione, 4-methoxy-7-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 32 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:560239 HCAPLUS
DOCUMENT NUMBER: 103:160239
TITLE: Chemistry of sulfur containing flavonoids
AUTHOR(S): Balint, J.; Bognar, R.; Rakosi, M.
CORPORATE SOURCE: Biogal Pharm. Works, Debrecen, H-4042, Hung.
SOURCE: Studies in Organic Chemistry (Amsterdam) (1985), 19(Org. Sulfur Chem.), 660-706
CODEN: SOCHDQ; ISSN: 0165-3253
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 316 refs.
IT **5465-04-3D**, derivs.
RL: RCT (Reactant); RACT (Reactant or reagent))
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 33 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:209579 HCAPLUS
DOCUMENT NUMBER: 100:209579
TITLE: Electrochemical synthesis of bipyranylidenes as a novel route to strongly donating systems
AUTHOR(S): Mabon, Gilles; Simonet, Jacques
CORPORATE SOURCE: Lab. Electrochim. Org., Univ. Cathol. Ouest, Angers, 49005, Fr.
SOURCE: Tetrahedron Letters (1984), 25(2), 193-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 100:209579
AB The electrochem. method is used in the easy synthesis of donating systems by means of the cathodic reduction of thiopyrones in the presence of alkyl halides. Thus, bipyranylidene I was prepared in 75% yield by electrochem. reduction of thiopyranone II in presence of Me3CBr.
IT **5465-04-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(electrochem. reductive coupling of)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)

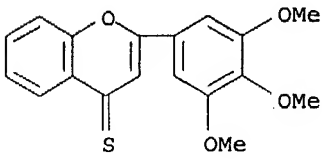


L32 ANSWER 34 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:53473 HCAPLUS
DOCUMENT NUMBER: 98:53473
TITLE: The preparation of flavones and their derivatives. Part I. Flavones and 4-thioflavones
AUTHOR(S): Briggs, Malcolm T.; Duncan, Graham L. S.; Thornber, Craig W.; Cooper, Christopher R.
CORPORATE SOURCE: Pharm. Div., ICI PLC, Macclesfield, SK10 4TG, UK
SOURCE: Journal of Chemical Research, Synopses (1982), (9), 242-3
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English

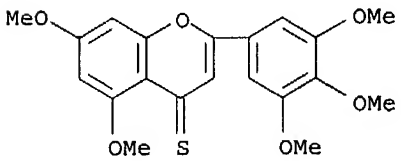
AB 5,7-Dihydroxyflavones were regioselectively alkylated at the 7-position using alkyl halides with K2CO3 in Me2CO or DMF whereas using NaH in DMF 5-alkylation was observed Condensation reactions of 2-hydroxyacetophenones with aroyl halides and esters followed by intramol. cyclocondensation of the resulting 1,3-diphenyl-1,3-propanediones gave flavones. 4-Thioflavones were prepared by thionation of the corresponding oxo derivs. with PS5 in THF. E.g., treatment of flavone I (Z = O) with PS5 in THF at room temperature for 1 h gave 96% thione I (Z = S).

IT **84212-79-3P 84212-81-7P 84212-83-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

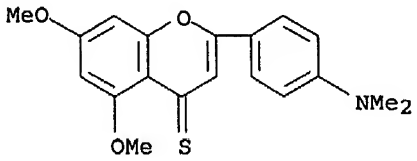
RN 84212-79-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



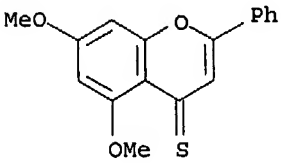
RN 84212-81-7 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



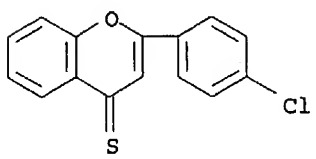
RN 84212-83-9 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-[4-(dimethylamino)phenyl]-5,7-dimethoxy- (9CI) (CA INDEX NAME)



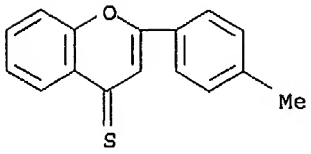
IT **84212-80-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by thionation of flavone)
RN 84212-80-6 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 5,7-dimethoxy-2-phenyl- (9CI) (CA INDEX NAME)



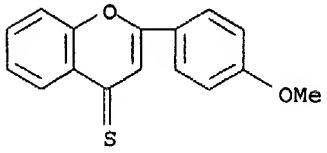
L32 ANSWER 35 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:438715 HCAPLUS
DOCUMENT NUMBER: 97:38715
TITLE: Reaction of hydroxylamine with 4'-substituted flavone derivatives
AUTHOR(S): Witczak, Zbigniew; Krolikowska, Maria
CORPORATE SOURCE: Inst. Fundam. Chem. Sci., Sch. Med., Lodz, 90145, Pol.
SOURCE: Polish Journal of Chemistry (1981), 55(4), 763-73
CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Flavones I (X = O, R = OMe, Me, Cl) reacted NH2OH to a give 3:1 mixture of II and I (X = NOH). Similar reaction of I (X = O, R = OH) gave only II (R = OH). Reaction of I (X = O, R = NO2) with NH2OH gave II (R = NO2), 3-(2-hydroxyphenyl)-5-(4-nitrophenyl)isoxazole, and 2-HOC6H4COCH:C(NHOH)C6H4NO2-4.
IT **16074-52-5P 16074-59-2P 82340-44-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with hydroxylamine)
RN 16074-52-5 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



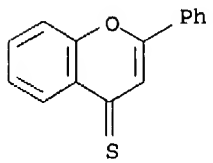
RN 16074-59-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



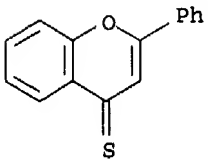
RN 82340-44-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L32 ANSWER 36 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1981:595069 HCAPLUS
DOCUMENT NUMBER: 95:195069
TITLE: Thione photochemistry: on the formation of dipyranylidenes from pyranthiones
AUTHOR(S): Berenjian, Nader; De Mayo, Paul
CORPORATE SOURCE: Dep. Chem., Univ. West. Ontario, London, ON, N6A 5B7, Can.
SOURCE: Canadian Journal of Chemistry (1981), 59(17), 2612-16
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The irradiation of the pyranthione(I) was reinvestigated. The reaction proceeded through the (n,π*) triplet and was quenched with ferrocene. The reaction was sensitized with Michler's ketone or triphenylene. The elimination of S from 2 mols. of I to give the dipyranylidene(II) required a H donor solvent, and the quantum yield of product increased with greater dilution because of the well-known quenching of triplet thiones by the ground state thione. A mechanism for the formation of II is suggested.
IT **5465-04-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(photolysis of, product formation in, mechanism of)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)

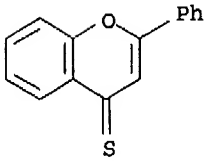


L32 ANSWER 37 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1980:199739 HCAPLUS
DOCUMENT NUMBER: 92:199739
TITLE: Pyrylocyanines. 9. Isobenzopyrylocyanines
AUTHOR(S): Tolmachev, A. I.; Shulezhko, L. M.
CORPORATE SOURCE: Inst. Org. Khim., Kiev, 252660, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1980), (2), 193-8
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 92:199739
AB 1-Methyl-3-phenyl-2-benzopyrylium perchlorate (I) [7654-71-9] was prepared by reaction of 3-phenylisocoumarin [4809-08-9] with MeMgI and used to prepare monomethine and carbocyanine dyes, either by direct reaction with anilinovinyl derivs. of quaternary heterocyclic bases or via 1-(formylmethylene)-3-phenyl-2-benzopyran [73589-88-5]. The sym. and unsym. isobenzopyrylocyanines prepared absorb at somewhat shorter wavelength than the isomeric flavylocyanines. In the sym. case, the vinylene shift from mono- to trimethine chain is .apprx.100 nm, which indicates the absence of steric hindrance in the monomethine. An analogous series of cyanines could not be obtained from the isomeric 3-methyl-1-phenyl-2-benzopyrylium perchlorate [73585-73-6].
IT **5465-04-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylphenylbenzopyrylium perchlorate)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)

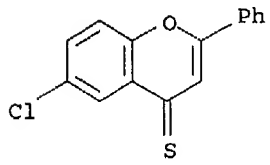


L32 ANSWER 38 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1979:137624 HCAPLUS
DOCUMENT NUMBER: 90:137624
TITLE: Silver and mercuric salts as catalysts in the reaction of 4-thionflavone and N-methyl-N-tosylhydrazine
AUTHOR(S): Cacchi, Sandro; La Torre, Francesco; Misiti, Domenico
CORPORATE SOURCE: Cattedra Chim. Org., Rome, Italy
SOURCE: Chemistry & Industry (London, United Kingdom) (1978), (17), 669-70
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 90:137624
AB In the presence of Hg(OAc)2, the title flavone I (Z = S) underwent condensation reaction with p-MeC6H4SO2NMeNH2 (II) to give 50% I (Z = p-MeC6H4SO2NMeN) (III) and 44% I (Z = O). The formation of I (Z = O) and III involves a common S-Hg coordinated intermediate. III was obtained (95%) by reaction of I (Z = S) with II in the presence of AgNO3.
IT **5465-04-3**

RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with methyl(tolylsulfonyl)hydrazine, silver and mercuric salt-catalyzed)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 39 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:436462 HCAPLUS
DOCUMENT NUMBER: 89:36462
TITLE: A new class of antimalarial drugs: derivatives of benzothiopyrans
AUTHOR(S): Razdan, Raj K.; Bruni, Robert J.; Mehta, Avinash C.; Weinhardt, Klaus K.; Papanastassiou, Zinon B.
CORPORATE SOURCE: Arthur D. Little, Inc., Cambridge, MA, USA
SOURCE: Journal of Medicinal Chemistry (1978), 21(7), 643-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 89:36462
AB Thirty-nine substituted benzothiopyrans I [R = (CH2)3NMe2, pyridyl, adamantyl, etc; R1 = Ph, p-ClC6H4, 3,4-dichlorophenyl, etc.; R2 = H, Cl, Br, F, or OMe] were synthesized by condensation of thiophenols with benzoylacetates, conversion of the resulting thioflavones to thionothioflavones, and treatment of these thionothioflavones or gem-dichloro intermediates with various primary amines. Some of the compds. had antimalarial activity and were curative at 160-360 mg/kg againt Plasmodium berghei in mice. Structure-activity relations are discussed.
IT **59835-95-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with dimethylpropanediamine)
RN 59835-95-9 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-chloro-2-phenyl- (9CI) (CA INDEX NAME)

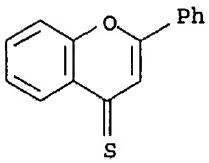


L32 ANSWER 40 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:62265 HCAPLUS
DOCUMENT NUMBER: 88:62265
TITLE: Flavonoids, XXXII. Oxidative transformation of

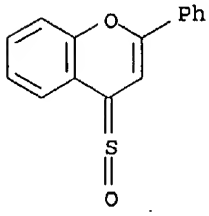
flavonoids containing sulfur
AUTHOR(S): Bognar, Rezso; Balint, Janos; Rakosi, Miklos
CORPORATE SOURCE: Inst. Org. Chem., Lajos Kossuth Univ., Debrecen, Hung.
SOURCE: Justus Liebigs Annalen der Chemie (1977), (9), 1529-35
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 88:62265

AB Oxidation of the flavenethione I (X = O, Z = S) and the thioflavenethione I (X = Z = S) with equimolar amts. of monoperoxyphthalic acid gave I (X = O, S; Z = SO), which were further oxidized to I (X = O, S; Z = O), I (X = O, S; Z = O) were also prepared by acid-catalyzed reaction of I (X = O, S; Z = S) with Me2SO. The preparation and reactions of I (X = SO, SO2; Z = O) and the thiaflavanones II (n = 0,1,2) were also investigated. II (n = O) and (NH4)2[Ce(NO3)6] gave I (X = S, Z = O) in 90% yield.

IT **5465-04-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)

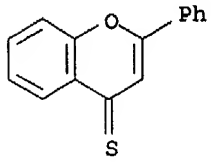


IT **65373-79-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
RN 65373-79-7 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl-, S-oxide (9CI) (CA INDEX NAME)

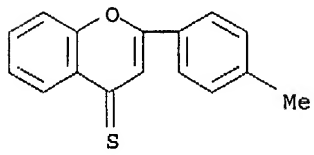


L32 ANSWER 41 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:6658 HCAPLUS
DOCUMENT NUMBER: 88:6658
TITLE: 8-Oxoheptafulvene. VIII. Synthesis of iso-π-electronic heteroanalogs of heptafulvalene
AUTHOR(S): Kato, Kazuo; Kitahara, Yoshio; Morita, Noboru; Asao, Toyonobu
CORPORATE SOURCE: Fac. Sci., Tohoku Univ., Sendai, Japan
SOURCE: Chemistry Letters (1977), (8), 873-6
CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:6658
AB Ten iso-π-electronic oxa- and thia-hetero analogs of heptafulvalene, such as I (R = H, Me, Ph, CO2Me; Z1 = Z), II (Z1 = Z), and III (R = H, CO2Me; Z1 = Z), were prepared by treating the corresponding I (Z1 = O, S), II (Z1 = O,S) and III (Z1 = S) with Z:C:O. These fulvalenes were polyolefinic by comparison of their NMR spectra with that of heptafulvalene.
IT **5465-04-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with 8-oxoheptafulvene)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)

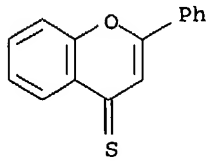


L32 ANSWER 42 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:484773 HCAPLUS
DOCUMENT NUMBER: 87:84773
TITLE: Reaction of 2'-hydroxy-4-methylchalcone with hydroxylamine hydrochloride
AUTHOR(S): Krolikowska, Maria; Witczak, Zbigniew
CORPORATE SOURCE: Dep. Org. Chem., Sch. Med., Lodz, Pol.
SOURCE: Roczniki Chemii (1977), 51(3), 611-15
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Reaction of o-HOC6H4COCH:CHC6H4Me-p with NH2OH.HCl yielded 5 compds. depending on reaction conditions; the main product was 4'-methylflavanone oxime (I).
IT **16074-59-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxylamine hydrochloride)
RN 16074-59-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methylphenyl)- (9CI) (CA INDEX NAME)

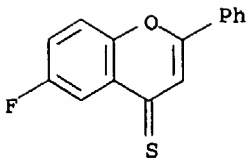


L32 ANSWER 43 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:439374 HCAPLUS
DOCUMENT NUMBER: 87:39374
TITLE: Reaction of 4-methoxy-1-benzopyrylium,

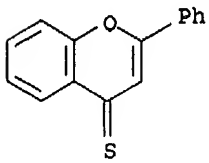
-benzothiopyrylium, and -benzoselenopyrylium salts with some nucleophilic agents
AUTHOR(S): Tolmachev, A. I.; Kudinova, M. A.; Shulezhko, L. M.
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1977), (2), 178-81
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Onium salts I, II, III [R = CH:CHCH:C(OMe)C6H4OAc-o] were obtained in 30-40% yields by heating IV (X = O) with the corresponding heterocyclic onium compound in AcOH 3 h at 100°. Analogously IV (X = Se) heated with 2-methylene-3-methylbenzothiazoline followed by treatment with HClO4 gave 10% V.
IT **5465-04-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylmethoxybenzopyrylium perchlorate)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



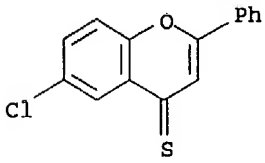
L32 ANSWER 44 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:446315 HCAPLUS
DOCUMENT NUMBER: 85:46315
TITLE: Synthesis and pharmacological activity of some derivatives of 4-imino- and oximinoflavenes
AUTHOR(S): Meshcheryakova, L. M.; Tsikalova, T. S.; Orlova, E. K.; Burov, Yu. V.; Speranskaya, N. P.; Zagorevskii, V. A.
CORPORATE SOURCE: Nauchno-Issled. Inst. Farmakol., Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1976), 10(3), 37-41
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 85:46315
AB Flavone O-alkyloximes [I, R = H, Cl, F, R1 = Me, PhCH2, p-O2NC6H4, Me2NCH2CH2, Et2NCH2CH2, Me2N(CH2)3, 4-methyl-1-piperazinylpropyl], useful as sedatives and in treatment of ataxia, were prepared in 40-85% yields by alkylation of the corresponding oximes with R1Cl. II (R = H, Cl) were obtained by treatment of a 4-thioflavone with H2NCH2CH2NMe2.
IT **59835-96-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 59835-96-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-fluoro-2-phenyl- (9CI) (CA INDEX NAME)



IT **5465-04-3 59835-95-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with N,N-dimethylethylenediamine)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)

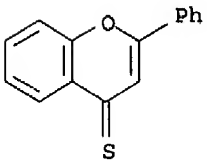


RN 59835-95-9 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-chloro-2-phenyl- (9CI) (CA INDEX NAME)

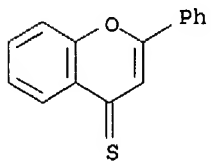


L32 ANSWER 45 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:179073 HCAPLUS
DOCUMENT NUMBER: 84:179073
TITLE: Carbon-13 nuclear magnetic resonance spectra of organic sulfur compounds. III. Comparison of chemical shifts for carbonyl and thiocarbonyl compounds in the pyrone, thiopyrone, and pyridone series
AUTHOR(S): Still, I. W. J.; Plavac, N.; McKinnon, D. M.; Chauhan, M. S.
CORPORATE SOURCE: Dep. Chem., Univ. Toronto, Toronto, ON, Can.
SOURCE: Canadian Journal of Chemistry (1976), 54(2), 280-9
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 13C NMR data are obtained for a series of 2- and 4-pyrones and pyridones, and their S-containing analogs. Correlations are observed between the nature of the ring hetero atom and the chemical shift difference ($\Delta\delta$) for the Cα and Cβ carbons in these conjugated systems. No significant correlation, however, exists between the chemical shifts of the C = (O) C = (S) groups. Substituent chemical shift effects for various simple

substituents are compared with those in related series of compds.
IT **5465-04-3**
RL: PRP (Properties)
(carbon-13 NMR spectrum of)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 46 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:37113 HCAPLUS
DOCUMENT NUMBER: 84:37113
TITLE: Carbon-13 nuclear magnetic resonance spectra of organic sulfur compounds. Cyclic sulfides, sulfoxides, sulfones, and thiones
AUTHOR(S): Chauhan, M. S.; Still, I. W. J.
CORPORATE SOURCE: Dep. Chem., Univ. Toronto, Toronto, ON, Can.
SOURCE: Canadian Journal of Chemistry (1975), 53(19), 2880-90
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 13C chemical shift data were obtained for >50 thiochromanones and related sulfoxide and sulfone derivs. The assignments of the various resonances in the most important of these were made by using the limited data already available and also by comparison with certain model compds., such as thioanisole, diphenyl sulfide, and the corresponding sulfoxides and sulfones. Within each of these 3 series and in a 4th which comprises derivs. of thiochromone, including 3 α,β-unsatd. thiones, the effects were examined on 13C chemical shift of substitution at varius positions in the thiochromanone skeleton. Among the substituents examined in this context are Me, Ph, methoxy, Br and carbomethoxy. Attempts to compare the 13C chemical shifts for the thiochromanone series with those in a few O-containing analogs and in a small number of structurally similar analogs are also discussed.
IT **5465-04-3**
RL: PRP (Properties)
(NMR of carbon-13 in)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



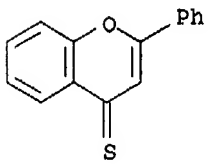
L32 ANSWER 47 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1975:85927 HCAPLUS
DOCUMENT NUMBER: 82:85927
TITLE: Proton-acceptor capability during the formation of hydrogen bonds in γ-pyrone compounds
AUTHOR(S): Tolmachev, A. I.; Papp, L. V.; Ryl'tsev, E. V.; Egorov, Yu. P.
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR
SOURCE: Zhurnal Obshchei Khimii (1974), 44(12), 2747-53
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB H bonding of PhOH with 23 pyran, selenopyran, and thiopyran 4-oxo, -selenoxo, and -thioxo derivs. was correlated with structure by ir spectroscopy. The oxo derivs. formed stronger H bonds than the selenoxo and thioxo derivs.; similarly the pyrans formed stronger H bonds than did the seleno- and thiopyrans.

IT **5465-04-3**
RL: PRP (Properties)
(hydrogen bonding of, with phenol, ir in relation to)

RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 48 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1974:146022 HCAPLUS
DOCUMENT NUMBER: 80:146022
TITLE: 4-Thiochromones
INVENTOR(S): Umio, Suminori; Ueda, Ikuo; Sato, Yoshinari; Matsuo, Masaaki
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

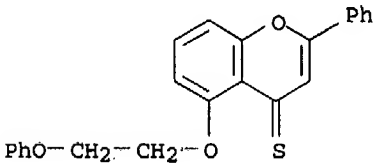
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 49024966	A2	19740305	JP 1972-65572	19720629
JP 56035673	B4	19810819		

PRIORITY APPLN. INFO.: JP 1972-65572 A 19720629
OTHER SOURCE(S): CASREACT 80:146022

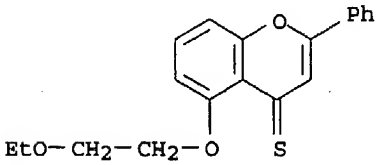
AB The antiallergic title compds. (I, R1 = aryl; R2 = alkoxy substituted with aryloxy or with alkoxy) were prepared by sulfurixing the chromones II. E.g., 0.8 g II [R1 = 2-Ph, R2 = 5-(2-phenoxyethoxy)] in C6H6 was refluxed 4 hr with 0.4 g P2S5 to give 0.5 g corresponding I. Similarly prepared was I [R1 = 2-Ph, R3 = 5-(2-ethoxyethoxy)].

IT **52578-43-5P 52578-44-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 52578-43-5 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 5-(2-phenoxyethoxy)-2-phenyl- (9CI) (CA INDEX NAME)

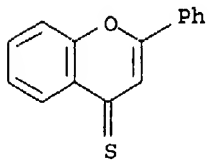


RN 52578-44-6 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 5-(2-ethoxyethoxy)-2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 49 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1971:455977 HCAPLUS
DOCUMENT NUMBER: 75:55977
TITLE: Electronic spectra and structure of γ-pyrone series compounds. III. Luminescence
AUTHOR(S): Efimov, A. A.; Nurmukhametov, R. N.; Belaits, I. L.; Tolmachev, A. I.
CORPORATE SOURCE: USSR
SOURCE: Optika i Spektroskopiya (1971), 30(4), 622-7
CODEN: OPSPAM; ISSN: 0030-4034
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The phosphorescence spectra of chromone (I), 7-methylchromone (II), flavone (III), isoflavone (IV), 7,8-benzoflavone (V), and 7,8-benzothioflaveone (VI) were measured in hydrocarbons and EtOH solns. at 77°K are presented in graphs. The spectra are located in the visible regions. No fluorescence was detected and this is caused by high probability of intercombination conversion. I and II in hydrocarbon solution exhibit short-lived nπ* phosphorescence (lifetime τ = .apprx.5 + 10-4 sec in both cases), but in EtOH solution show long-lived ππ* phosphorescence (τ = 0.43 and 0.40 sec, resp.). The nπ* band is of quasilinear structure and exhibits the carbonyl frequency (1665 ± 15 cm-1) progression. III-VI show long-lived ππ* phosphorescence in hydrocarbon as well as in EtOH solns. This is related to their more extended π-electron system as compared with that of I and II. The ππ*-phosphorescence band of III and V is blue shifted by .apprx.500 cm-1 on passing from hexane to alc. solution The relative locations of singlet and triplet nπ*- and ππ*-levels for I-VI and γ-pyrone and xanthone (VII) are presented in diagrams. The value of S*, T-splitting of nπ*-level of γ-pyrone compds. is estimated on the basis of data for I, II, and VII as .apprx.1500-2500 cm-1.

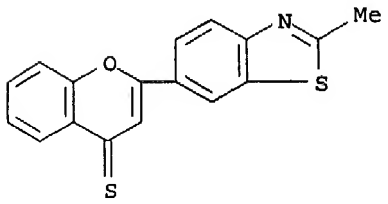
L32 ANSWER 50 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1971:412884 HCAPLUS
DOCUMENT NUMBER: 75:12884
TITLE: Ultraviolet absorption spectroscopic investigation and the relative basicity of thioflavonoid compounds. II
AUTHOR(S): Rakosi-David E.; Rakosi, Matej; Balint, J.; Bognar, R.
CORPORATE SOURCE: Szerves Kem. Intez., Kossuth Lajos Tud. Egy., Debrecen, Hung.
SOURCE: Acta Physica et Chimica Debrecina (1970), 15/16, 163-80
CODEN: APDBAN; ISSN: 0567-7947
DOCUMENT TYPE: Journal
LANGUAGE: German
AB The uv spectra of 1-thiaflavanone (I), I oxime, 3-amino-1-thiaflavanone hydrochloride, 3-bromo-1-thiaflavanone (II), 1-thiaflavone (III), III oxime, 4-thioflavone, 1-thia-4-thioflavone, 3-amino-1-thiaflavone, β-4-hydroxy-1-thiaflavan, and 4-amino-1-thiaflavan, were investigated and compared with those of the corresponding O analogs. The substitution of 1-O, of the carbonyl O, and both of O atoms, resp., for S resulted in a shift (20-40 nm, 100 nm, and 150 nm, resp.) of the bands. The relative basicity consts. (pKBH+) of the above compds. were calculated, and the relations: CO > CS and O < S were found. The rate of the elimination of HBr from II was increased by the effect of the unshared electrons of the S atom in the ring in comparison to that of the O analog.
IT **5465-04-3**
RL: PRP (Properties)
(basicity and uv spectrum of)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 51 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1970:510856 HCAPLUS
DOCUMENT NUMBER: 73:110856
TITLE: Chromonylbenzothiazoles and cyanine dyes made from them
AUTHOR(S): Tolmachev, A. I.; Belaya, Zh. N.
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR
SOURCE: Khim. Str., Svoistva Reaktivnost Org. Soedin. (1969), 38-44. Editor(s): Kuprianov, A. I. Izd. "Naukova Dumka": Kiev, USSR.
CODEN: 17JAAD
DOCUMENT TYPE: Conference
LANGUAGE: Russian
AB 2-Methyl-x-benzothiazolecarbonyl chloride and 4,2-X(HO)C6H4Ac (I, X = H, MeO), 2,1- or 1,2-HOC10H6Ac in pyridine form the corresponding esters (II), which undergo the Baker-Venkataraman rearrangement in the presence of KOH in pyridine solution to give III, which are cyclized to chromonylbenzothiazoles (IV) by H2SO4 in CHCl3. IV form quaternary salts

(V) with R5I in PhNO2. Use of R2SSO4 and of RSO3R5 led to deeply colored products. The following II-V were prepared (R1-R5, x, Y, and m.p. of II-V given): H, H, H, H, Et, 5, iodide, 108°, 165°, 215°, 280°; H, H, H, H, Me, 6, ClO4, 141°, 137°, 203°, 267°; H, H, MeO, H, Me, 6, ClO4, 115°, 176°, 216°, 244°; (R1R2 =) benzo, H, H, Me, 6, ClO4, 160°, 80°, 260°, 250°; H, H, (R3R4 =) benzo, Me, 6, iodide, 174°, 209°, 249°, 245°. Reaction of IV (R1-R4 = H, x = 6) (VI) with P2S5 in benzene gave VII (Z = S), m. 258°. Heating 0.293 g VI with 0.066 g CH2(CN)2 and 1 ml Ac2O for 3 hr at 135° gave VII [Z = C(CN)2], m. 293° (MeOHMeNO2). VIII, m. 280° (decomposition), λmaxEtOH 492 mμ, was obtained by treating VI with 2,3-dimethylbenzothiazolium Me sulfate in Ac2O for 3 hr at 130°. Treating IV.EtI with HC(OEt)3 in PhNO2 at 190° gave the following IX [R1-R4, x, m.p. (decomposition), and λmaxEtOH (mμ) given]: H, H, H, H, 5, 317° (HOAc), 570; H, H, H, H, 6, 305° (HOAc), 594; H, H, MeO, H, 6, 290° (HOAc), 594; (R1R2 =) benzo, H, H, 319° (MeNO2), 594; H, H, (R3R4 = benzo), 326° (PhNO2), 594. VI.p-MeC6H4SO3Et reacted with 3-ethyl-2-(ethylthio)benzothiazolium Et sulfate to give X (n = 0, x = 6, Y = ClO4), m. 279° (decomposition) (EtOH), λmaxEtOH 442 mμ. The appropriate IV.EtI reacted with 3-ethyl-2-(2-acetanilidovinyl)benzothiazolium tosylate to give X (n = 1, Y = iodide) [x, m.p. (decomposition) (HOAc), and λmaxEtOH (mμ) given]: 5, 296°, 564; 6, 280°, 578. The same compds. by conventional means gave XI and XII [x, m.p. (decomposition) and λmaxEtOH (mμ) of XI, and m.p. (decomposition) (EtOH) and λmaxEtOH (mμ) of XII given]: 5, 360° (C5H5N-EtOH), 525, -, -; 6, 310° (HOAc), 538, 260°, 563. The shift in absorption produced by chromonyl substituents is quite similar to that produced by the benzothiazolyl group.

IT **29808-31-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 29808-31-9 HCAPLUS
CN Chromone, 2-(2-methyl-6-benzothiazolyl)-4-thio- (8CI) (CA INDEX NAME)



L32 ANSWER 52 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:524118 HCAPLUS
DOCUMENT NUMBER: 71:124118
TITLE: Silicon disulfide and boron sulfide in the preparation of thiones and pyranthiones
AUTHOR(S): Dean, Francis M.; Goodchild, J.; Hill, Andrew William
CORPORATE SOURCE: Univ. Liverpool, Liverpool, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1969), 16, 2192-5
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal

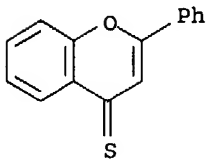
LANGUAGE: English

AB Silicon disulfide and boron sulfide can be used with advantage instead of P2S5 for converting non-enolizable ketones, 2-pyrones, and 4-pyrones into the corresponding thiones. Of the three reagents, boron sulfide is the most active and is often effective at ordinary temps. A convenient synthesis of 3,4-benzocoumarin is noted.

IT **5465-04-3P 24051-70-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

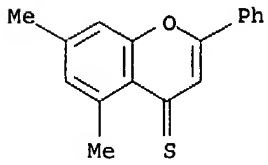
RN 5465-04-3 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



RN 24051-70-5 HCAPLUS

CN Flavone, 5,7-dimethyl-4-thio- (8CI) (CA INDEX NAME)



L32 ANSWER 53 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1969:114945 HCAPLUS

DOCUMENT NUMBER: 70:114945

TITLE: α-Halo ethers. XL. Flavonoids. 17. Preparation and reactions of some 4,4-dichloroflavene derivatives

AUTHOR(S): Farkas, Istvan; Costisella, Burkhard; Rakosi, Miklos; Gross, Hans; Bognar, Rezso

CORPORATE SOURCE: Univ. Debrecen, Debrecen, Hung.

SOURCE: Chemische Berichte (1969), 102(4), 1333-8
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

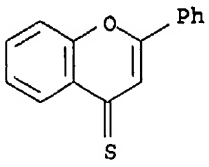
LANGUAGE: German

AB Treatment of 2-phenyl-7-(R-substituted)-flavones (I, where R = H, AcO, or tetracetyl-β-D-glucopyranosyloxy) with MeOCHCl2 gave 2-phenyl-4,4-dichloro-7-(R-substituted)-2-flavenes (II). The dichloro derivs. of 3-acetoxyflavone, 3-methoxyflavone, and 3,3',4',5,7-pentacetoxyflavone could not be prepared by this method. Treatment of II with AcSH in C6H6 gave 2-phenyl-7-(R-substituted)thioflavones. II (R = H) reacted with MeOH to give I (R = H), with PhSH to give 2-phenyl-4,4-bis(phenylthio)-2-flavene and with R1NH2 to give 2-phenyl-4-(R1N:-substituted)-2-flavene (where R = Ph, C10H21, or OH). 2-Phenylthioflavone reacted similarly to I.

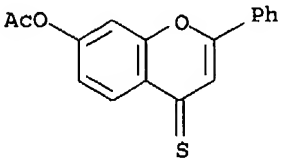
IT **5465-04-3P 22115-91-9P 22145-03-5P 22145-04-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)

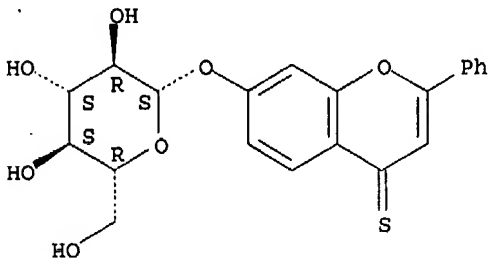


RN 22115-91-9 HCAPLUS
CN Flavone, 7-hydroxy-4-thio-, acetate (8CI) (CA INDEX NAME)



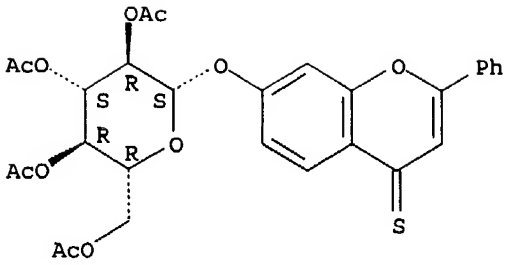
RN 22145-03-5 HCAPLUS
CN Flavone, 7-hydroxy-4-thio-, β-D-glucopyranoside (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 22145-04-6 HCAPLUS
CN Flavone, 7-hydroxy-4-thio-, β-D-glucopyranoside tetraacetate (8CI) (CA INDEX NAME)

Absolute stereochemistry.



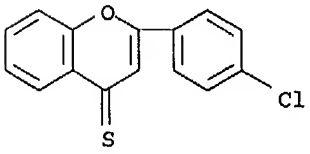
L32 ANSWER 54 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1967:508619 HCAPLUS
DOCUMENT NUMBER: 67:108619
TITLE: Heterocyclic sulfur compounds. XXVIII. Action of phosphorus pentasulfide on β,δ-diketophenols
AUTHOR(S): Stavaux, Madeleine; Lozac'h, Noel
CORPORATE SOURCE: Fac. Sci., Caen, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1967), (6), 2082-90
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 67:108619

AB cf. preceding abstrs. Compds. of the general formula RCOCHR1COCHR2COR3 (I) are treated with P2S5 to give compds. of the general formulas II and III. Similarly, compds. of the general formulas o-(ArCOCH2CO)C6H4OH (IV) and 2-HOC10H6COCH2COAr-1 (V) give compds. of the general formulas VI, VII, VIII, and IX. An acetylacetone-BzOMe-NaH 1:1.2:4 molar mixture gives 58% 1-acetyl-3-benzoylacetone (IXa), m. 101°. A mixture of 4 g. IXa, 8 g. P2S5, and 500 ml. C6H6 is refluxed 1 hr. to give 28% II (R = Me, R1 = R2 = H, R3 = Ph), m. 169° (MeOH). Similarly prepared are the following I and II (R, R1, R2, R3, m.p. I, % yield I, m.p. II, and % yield II given): Me, H, H, p-MeOC6H4, 81°, 72, 221° (EtOAc), 55; Me, H, H, p-tolyl, 65, 89, 193° (EtOAc), 40; Ph, H, H, p-MeOC6H4, 120°, 85, 186° (C6H6), 42; Ph, H, H, 3-pyridyl, 96°, 63, 151° (EtOH), 26; Ph, H, H, PhCH:CH, 127°, 50, 233° (C6H6), 17; PhCH:CH, H, H, PhCH:CH, 168°, 67, 271° (HCONMe2), 5; Ph, Ph, H, Ph, 105-8°, 88, 188° (EtOAc), 30; Ph, Ph, Ph, Ph, 123°, 85, 262°, (C6H6), 5; Ph, Me, H, Ph, -, 78, 157° (EtOAc), 30; Ph, Me, Me, Ph, -, 68, 184° (cyclohexane), 10; Ph, Me, Ph, Ph, -, 57, 176° (cyclohexane), 15; Ph, (R1R2 =) CH2CH2, Ph, 123°, 86, 233° (C6H6), 26; p-MeOC6H4, (R1R2 =) CH2CH2, p-MeOC6H4, 173°, 66, 290° (EtOH-C6H6), 30; p-tolyl, (R1R2 =) CH2CH2, p-tolyl, 138-40°, 87, 246° (C6H6), 29; p-ClC6H4, (R1R2 =) CH2CH2, p-ClC6H4, 182°, 72, 254° (C6H6), 28; Ph, (R1R2 =) (CH2)3, Ph, 124°, 86, 153° (EtOH-C6H6), 22; p-MeOC6H4, (R1R2 =) (CH2)3, p-MeOC6H4, 155-7°, 56, 219° (C6H6), 30; p-tolyl, (R1R2 =) (CH2)3, p-tolyl, 178-80°, 76, 225° (C6H6), 30; p-ClC6H4, (R1R2 =) (CH2)3, p-ClC6H4, 181°, 61, 207° (C6H6), 16; Ph, (R1R2 =) CH2CHMeCH2, Ph, 161°, 84, 164° (EtOH-C6H6), 17; p-MeOC6H4, (R1R2 =) CH2CHMeCH2, p-MeOC6H4, (204°, 80, 209° (EtOH-C6H6), 15; p-tolyl, (R1R2 =) CH2CHMeCH2, p-tolyl, 207-8°, 82, 205° (EtOAc), 15. Incomplete sulfuration of the I gives the following III (n, Ar, m.p., and % yield given): 0, Ph,

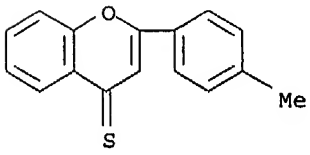
163°, 99; 0, p-MeOC6H4, 158°, 40; 0, p-tolyl, 178-80°, 61; 0, p-ClC6H4, 207°, 82; 1 (X = CH2), Ph, 175°, 22; 1 (X = CH2), p-MeOC6H4, 233°, 23; 1 (X = CH2), p-tolyl, 228°, 20; 1 (X = CH2), p-ClC6H4, 198°, 20; 1 (X = CHMe), Ph, 139°, 50; 1 (X = CHMe), p-MeOC6H4, 184, 40; 1 (X = CHMe), p-tolyl, 190-4°, 33. o-Hydroxyacetophenone is treated with a BzOH ester to give 60% IV (Ar = Ph) (X), m. 119-20°. Similarly prepared are the following IV (Ar, m.p., and % yield given): p-MeOC6H4, 113°, 77; p-tolyl, 108°, 56; p-ClC6H4, 125°, 66; PhCH:CH, 133°, 77. Similarly prepared are 1-benzoylacetyl-2-naphthol (V, Ar = Ph) (XI) (62%), m. 137°, and the following V (Ar, m.p., and % yield given): p-MeOC6H4, 102°, 50; p-tolyl, 117°, 60; p-ClC6H4, 147°, 75. A mixture of 4 g. X, 8 g. P2S5, and 200 ml. pyridine is refluxed 1 hr., the product chromatographed, and the column eluted to give 65% 2-phenylchromene-4-thione (VI, Ar = Ph), m. 83°; the column is then eluted to give 14% o-(5-phenyl-1,2-dithiole-3-ylio)phenoxide (VIII, Ar = Ph), m. 158°. Similarly prepared are the following VI and VIII (Ar, m.p. VI, % yield VI, m.p. VIII, and % yield VIII given): p-MeOC6H4, 137°, 61, 174°, 14; p-tolyl, 146°, 41, 185°, 15; p-ClC6H4, 197°, 22, 197°, 27; and VI (Ar = PhCH:CH) (35%), m. 164°. XI gives a mixture containing 33% 2-phenylbenzo[f]chromonene-4-thione (VII, Ar = Ph) (m. 149°) and 15% 1-(5-phenyl-1,2-dithiol-3-ylio)-2-naphthoxide (IX, Ar = Ph) (m. 150°). Similarly prepared are the following VII and IX (Ar, m.p. VII, % yield VII, m.p. IX and % yield IX given): p-MeOC6H4, 158°, 73, 158°, 15; p-tolyl, 189°, 58, 160°, 15; p-ClC6H4, 207°, 29, 155°, 9. 2,5-Diarylcyclopenta[c,d]-1,6,6aSIV-trithiapentalenes (200 mg.) are treated with 400 mg. Hg(OAc)2 in 50 ml. HOAc to give III (n = 0) where Ar = Ph, p-MeOC6H4, p-tolyl, and p-ClC6H4.

IT **16074-52-5P 16074-59-2P 16074-90-1P 16074-91-2P 16136-06-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 16074-52-5 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

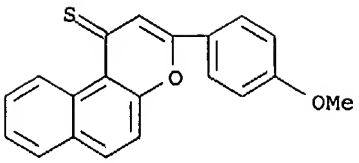


RN 16074-59-2 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-methylphenyl)- (9CI) (CA INDEX NAME)

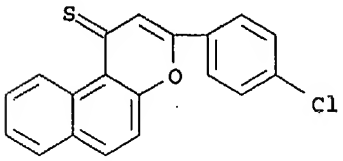


RN 16074-90-1 HCAPLUS
CN 1H-Naphtho[2,1-b]pyran-1-thione, 3-(p-methoxyphenyl)- (8CI) (CA INDEX

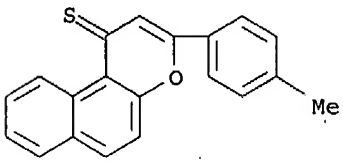
NAME)



RN 16074-91-2 HCAPLUS
CN 1H-Naphtho[2,1-b]pyran-1-thione, 3-(p-chlorophenyl)- (8CI) (CA INDEX NAME)



RN 16136-06-4 HCAPLUS
CN 1H-Naphtho[2,1-b]pyran-1-thione, 3-p-tolyl- (8CI) (CA INDEX NAME)

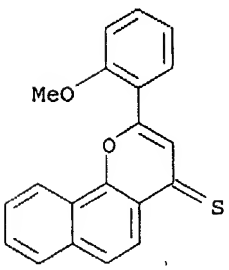


L32 ANSWER 55 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1967:454060 HCAPLUS
DOCUMENT NUMBER: 67:54060
TITLE: Heterocyclic sulfur compounds. XXV. Sulfuration of 2-(3-arylallylidene)-1-tetralones
AUTHOR(S): Poirier, Yves; Lozac'h, Noel
CORPORATE SOURCE: Fac. Sci. Caen, Caen, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1967), (3), 865-70
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
AB cf. preceding abstract Compds. of the general formula I are treated at .apprx.200° with S to give mixts. containing compds. of the general formula II (X = S) and III. Small dipole moment values are obtained for the III; the presence of O-S bonds (IV) is suggested. Thus, o-MeOC6H4CHO is condensed with AcH to give 57% o-MeOC6H4CH:CHCHO, b13 163-5°, m. 45-6°. Similarly prepared are the following ArCH:CHCHO (Ar, b.p./mm., and m.p. given): p-MeOC6H4, 170-5°/13, 57-9°; 2,3-(MeO)2C6H3, 160°/5, 77.5°; 3,4-(MeO)2C6H3, 170-90°/13, 81°; 3,4-methylenedioxyphenyl, 190-210°/12, 85°; p-tolyl, 154-9°/25, 41.5°;

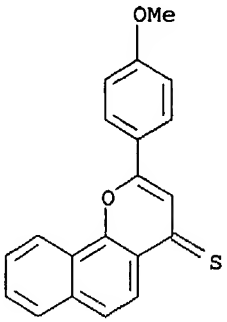
2-furyl, 105-10°/13, 51°; 2-thienyl, 95°/1, -. A mixture of 0.1 mole 1-tetralone, 0.12 mole PhCH:CHCHO, and 50 ml. 4% KOH (alc.) is kept 1 hr. to give I (Ar = Ph) (V), m. 134°. Similarly prepared are the following I (Ar and m.p. given): o-MeOC6H4, 130°; p-MeOC6H4, 146°; 2,3-(MeO)2C6H3, 123.5°; 3,4-(MeO)2C6H3, 129.5°; 3,4-(methylenedioxy)phenyl, 172°; p-tolyl, 152°; 2-furyl, 98°; 2-thenyl, 128°. A mixture of 20 g. V and 30 g. S is heated 1 hr. at 200-10° to give a mixture of 2-phenylbenzo[h]chromene-4-thione (II, Ar = Ph, X = S) (VI), 173.5°, and 2-(5-phenyl-1,2-dithiole-3-ylio)naphtholate (III, Ar = Ph) (VIa), m. 180°. Similarly prepared are the following II (X = S)-III mixts. (Ar, m.p. II, and m.p. III given): o-MeOC6H4, 177.5°, 139°; p-MeOC6H4, 224°, 218-19°; 2,3-(MeO)2C6H3, 149.5°, -; 3,4-(MeO)2C6H3, 203°, 179°; 3,4-(methylenedioxy)phenyl, 253°, 208°; p-tolyl, 190°, 186.5°, 2-furyl, 173°, 197-8°; 2-thienyl, 189°, 192.5°. VI is treated with KMnO4 to give 2-phenylbenzo[h]chromen-4-one (II, X = O, Ar = Ph), m. 154°. Similarly prepared are the following II (X = O) (Ar and m.p. given): o-MeOC6H4, 164°; p-MeOC6H4, 184°; 2,3-(MeO)2C6H3, 147° and 152.5°; 3,4-(MeO)2C6H3, 190°; 3,4-(methylenedioxy)phenyl, 261°; p-tolyl, 177°; 2-furly, 208°; 2-thienyl, 159°. A mixture of 3.5 g. 1-tetralone and 2.5 g. 3-phenyl-1,2-dithiolium perchlorate is heated to give 2-(5-phenyl-1,2-dithiole-3-ylidene)-1-tetralone (VII), m. 139° [perchlorate m. 209-10° (decomposition)]. A mixture of 100 mg. VII and 200 mg. S is heated 1 hr. at 200° to give III (Ar = Ph) (VIa). Similarly prepared are 2-[5-(p-methoxyphenyl)-1,2-dithiole-3-ylidene]-1-tetralone, m. 171°, and III (Ar = p-MeOC6H4). A mixture of 1.5 g. VII, 3 g. P2S5, and 80 ml. xylene is refluxed 1 hr. to give IVa, m. 158°.

IT **14756-13-9P 14756-14-0P 14756-15-1P 14756-16-2P 14756-17-3P 14756-18-4P 14882-98-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

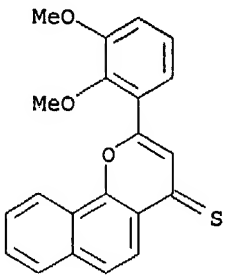
RN 14756-13-9 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-(o-methoxyphenyl)- (8CI) (CA INDEX NAME)



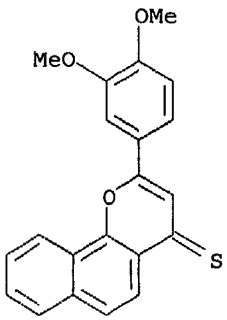
RN 14756-14-0 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-(p-methoxyphenyl)- (8CI) (CA INDEX NAME)



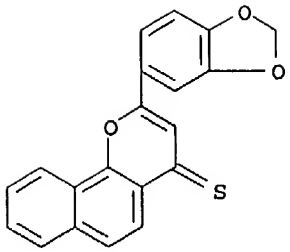
RN 14756-15-1 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-(2,3-dimethoxyphenyl)- (8CI) (CA INDEX NAME)



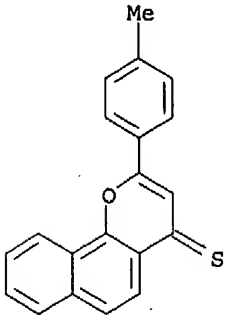
RN 14756-16-2 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-(3,4-dimethoxyphenyl)- (8CI) (CA INDEX NAME)



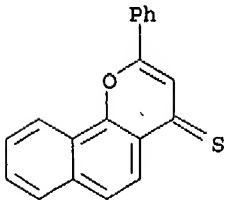
RN 14756-17-3 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-[3,4-(methylenedioxy)phenyl]- (8CI) (CA INDEX NAME)



RN 14756-18-4 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-p-tolyl- (8CI) (CA INDEX NAME)



RN 14882-98-5 HCAPLUS
CN 4H-Naphtho[1,2-b]pyran-4-thione, 2-phenyl- (8CI, 9CI) (CA INDEX NAME)



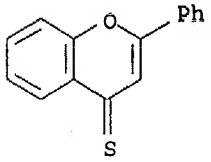
L32 ANSWER 56 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1966:8362 HCAPLUS
DOCUMENT NUMBER: 64:8362
ORIGINAL REFERENCE NO.: 64:1494e-h
TITLE: Ultraviolet absorption investigations on thioflavonoid compounds
AUTHOR(S): David, R. Eva; Bognar, Rezso; Rakosi, Miklos
CORPORATE SOURCE: Kossuth L. Tud. Egyet. Szerves Kem. Int., Debrecen, Hung.
SOURCE: Acta Physica et Chimica Debrecina (1965), Volume Date 1964, 10, 97-109
CODEN: APDBAN; ISSN: 0567-7947
DOCUMENT TYPE: Journal
LANGUAGE: German

AB The uv spectra of thioflavonoids were measured in absolute EtOH and compared with those of the corresponding O analogous basic compds. (λmaximum given in mμ and log ε are tabulated). Flavone: 302, 4.36; 252, 4.32; 214, 4.32. 1-Thiaflavone: 345, 4.2; 302+, 4.08; 272, 4.61. 4-Thionoflavone: 390, 4.28; 310, 4.28; 256+, 3.87; 236, 4.29. 1-Thia-4-thionoflavone: 425, 4.44; 320, 4.32; 260, 4.40; 240, 4.41. Flavanone: 320, 3.6; 252, 4.0. 1-Thiaflavanone: 350, 3.505; 256+, 3.86; 240, 4.47. Flavanone oxime: 312, 3.60; 255, 4.04. 1-Thiaflavanone oxime: 320, 3.37; 240, 4.251. 4-Aminoflavan: 286, 3.2; 274, 3.32. 4-Amino-1-thiaflavan: 258, 4.08; 294+, 3.14. 3-Aminoflavanone: 330, 3.56; 260, 4.04; 214, 4.4. 3-Aminoflavone: 373, 4.08; 308+, 3.72; 244, 4.32. β-4-Oxyflavan: 282, 3.2; 274, 3.4. β-4-Oxy-1-thiaflavan: 294+, 3.14; 258, 4.086. 3-Amino-1-thiaflavone: 352, 3.24; 270+, 3.60; 240, 4.2. 3-Amino-4-thionoflavone: 490, 4.4; 356, 4.08; 300+ 3.8; 242, 4.44. Flavone oxime: 341, 3.48; 278, 4.24; 242, 4.32. 1-Thiaflavone oxime: 359, 4.38; 312+, 4.12; 270, 4.60 (+ denotes inflections). The thioflavonoid compds. absorb in the regions of longer wavelength compared with the O analogs and, according to their intense color, in some cases they have absorption maximum also in the visible region. The degree of the bathochromic effect changes according to the extent that the O atom of the hetero ring, or that of the carbonyl group, or both were substituted for the S atom.

IT **5465-04-3**, Flavone, 4-thio-
(spectrum of)

RN 5465-04-3 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 57 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1965:66387 HCAPLUS

DOCUMENT NUMBER: 62:66387

ORIGINAL REFERENCE NO.: 62:11763h,11764a-h

TITLE: New thiochromone synthesis

AUTHOR(S): Bossert, Friedrich

CORPORATE SOURCE: Farbenfabriken Bayer Werk, Elberfeld, Germany

SOURCE: Justus Liebigs Annalen der Chemie (1964), 680, 40-51
CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 62:66387

AB Condensation of thiophenols with β-oxo carboxylic acid esters in polyphosphorie acid (I) yielded up to 90% corresponding thiochromones. The appropriate thiophenol (0.1-0.15 mole) in 0.12-0.18 mole β-oxo ester added dropwise with stirring at 80-90° during 10-15 min. to about 300 g. I, heated 15-30 min., and poured onto ice gave the corresponding thiochromone in 80-90% yield. H3PO4 (d. .apprx.1.75)(700 cc.) and 1.3 kg. P2O5 treated dropwise at 80-90° with 100 cc. PhSH in 210 cc. BzCH2CO2Et and kept 20-30 min. at 90-100° yielded 200 g. thioflavone, m. 124-6°. Similarly were prepared the following substituted thiochromones [substituent(s) and m.p. given]: 2-methyl,

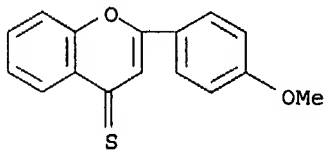
105° (C6H6-ligroine)(b0.01 140-5°); 3-methyl, 105° (ligroine); 2,6-dimethyl, 122° (C6H6-ligroine); 2,8-dimethyl, 125° (MeOH); 2-methyl-3-heptyl, 43-5° (b3 194-8°); 2,5,8-trimethyl, 89-90° (ligroine); 2-methyl-6-chloro (40-50% yield), 170° (EtOH); 2-methyl-8-chloro, 152° (ligroine); 2-methyl-6-bromo (40-50% yield), 176° (EtOH); 2-methyl-6-amino, 256-8°; 2-methyl-8-nitro, 192-3° (ligroine); 2-methyl-8-carbethoxyamino, 174° (C6H6-ligroine)(from o-EtO2CNHC2H4SH, b4 144°); 2-methyl-8-amino, 156-8° (C6H6-ligroine); 2-methyl-8-carbomethoxy, 1246° (MeOH); 2-methyl-5,8-dichloro, 124° (MeOH); 2,8-dimethyl-5-chloro, 130° (ligroine); 2-methyl-5-chloro-8-methoxy, 163-4° (MeOH)[from 5,2-Cl(MeO)C6H3SH, m. 40-2°]; 2-methyl-5-acetamido-8-chloro, 192° (EtOH)[from 2,5-Cl(AcNH)C6H3SH, m. 97-8° (C6H6-ligroine)]; 2-methyl-5-amino-8-chloro, 179-80° (EtOH); 2-methyl-3-(2-hydroxyethyl), 152° (EtOH); 2-methyl-3-(2-hydroxyethyl)-6-chloro, 42-4° (b0.1, 190-5°); 2,8-dimethyl-3-(2-hydroxyethyl)-5-chloro, 65° (b0.1 184-6°); 2-methyl-3-(2-hydroxyethyl)-8-carbomethoxy, 108-10° (EtOH)[free acid m. 202-4° (EtOH)]; 2-carbethoxy, 99-100° (C6H6-ligroine)[free acid m. 234° (EtOH)]; 6-chloro-2-carboxy (in 10% yield by the saponification of the crude Et ester), 253° (EtOH); 5-methyl-8-methoxy-2-carbethoxy (20% yield), 118° (MeOH); 2-carboxy-5-methyl-8-methoxy, 237-8° (EtOH); 2-carbethoxy-5-methyl-8-methoxy, 92° (ligroine); 2-carbethoxymethyl-5-methyl-8-methoxy, 100-1° (EtOH); 2-cyclohexyl-5-methyl-8-methoxy, 174°, (C6H6-igroine); 2-(4-pyridyl)-6-chloro, 207° (EtOH); 2-(4-pyridyl)-8-methoxy, 222° (EtOH); 2-(2-furyl)-5-methyl-8-methoxy, 167-8° (MeOH); 2-(2-thienyl)-5-methyl-8-methoxy, 153-4° (EtOH). Similarly were prepared the following substituted 2-phenylthiochromones (same data given): 6-Me, 154° (EtOH); 8-Me, 124° (EtOH); 6-MeO, 157° (EtOH); 7-MeO, 150° (MeOH); 8-Cl, 168° (EtOH); 8-EtO2CNH, 175-6° (C6H6-ligroine); 8-NH2, 139-41° (C6H6); 8-MeO2C, 126° (MeOH); 8-carbomethoxy-6-chloro-4'-methoxy, 196-8° (EtOH); 3'-NO2, 176° (EtOH); 4'-NO2, 183° (EtOH); 4'-MeO, 145-7° (C6H6); 6-chloro-4'-nitro, 240° (EtOH); 6-chloro-4'-methoxy, 179-81° (EtOH); 4',6-dichloro, 202-4° (EtOH); 4'-chloro-5-methyl-8-methoxy, 199-200° (EtOH); 5-amino-8-chloro, 156-8° (EtOH)[from 5-acetamido-8-chlorothioflavone, m. 162° (EtOH)]; 5-amino-8-chloro-4'-methoxy, 162-4° (C6H6-ligroine)[from 5-acetamido-8-chloro-4'-methoxythioflavone, m. 188-90° (EtOH)]; 8-carbomethoxy-4'-methoxy, 205° (EtOH). Similarly were prepared the following II (R, n, and m.p. given): 8-MeO, 3, 131° (EtOH); 8-CO2Me, 3, 191° (MeOH); 8-carbomethoxy-6-chloro, 3, 208° (EtOH); 6-Me2N, 4, 106° (MeOH); 8-EtO2CNH, 4, 182° (C6H6); 8-NH2, 4, 216-18° (EtOH); 5-chloro-8-methoxy, 4, 150-2° (EtOH); 5-acetamido-8-chloro, 4, 179-80° (EtOH); 6-Cl, 5, 100° (EtOH); 5-amino-8-methyl, 5, 172° (EtOH). PhSH (200 g.) treated dropwise at 60-70° in the presence of a small amount of NaOMe with 210 g. CH2:CMeCO2Me and heated 1 hr. at 80°, and the resulting PhSCH2CHMeCO2Me, b4 133°, refluxed 12 hrs. with 3.5. l. 6N HCl gave nearly quant. PhSCH2CHMeCO2H, m. 50°. Similarly were prepared 90% PhSCHMeCH2CO2H, b4 165°, and 85% 2,5-Me2C6H3SCH2CHMeCO2H, b3 185°. PhSH added to di-Me maleate yielded nearly quant. the di-Me ester of PhSCH(CO2H)CH2CO2H (III), b5 170°, which hydrolyzed yielded III, m. 117°. PhSCH2CHMeCO2H (300 g.) in 1.5 l. concentrated H2SO4 stirred 2 hrs. at room temperature gave 180 g. 3-methylthiochromanone (IV), b5 132°. IV (105 g.) in 2.3 l. C6H6

refluxed 0.5 hr. with 380 g. PCl5 gave 46 g. 3-methylthiochromone, m. 104-5° (1:1 H2O-MeOH). Similarly were prepared 2-methylthiochromanone, b4 128°, and 2-methylthiochromone, m. 105° (C6H6-ligroine), 70% 2,5,8-trimethylthiochromanone, b3 140°, and the thiochromone analog, m. 88-98° (ligroine), 80% 2,6-dimethyl-5-chlorothioehromanone, b3 163°, and the thiochromone analog, m. 130-1°. 2-Carboxythiochromanone was converted to the Et ester, b5 182-3°, in 90% yield, which gave similarly 50% 2-carbethoxythiochromone, m. 99-100°.

IT **82340-44-1**, Thioflavone, 4'-methoxy- **140885-77-4**, Thioflavone, 6-methyl- **140885-99-0**, Thioflavone, 8-methyl- **244107-94-6**, Thioflavone, 7-methoxy- **256464-73-0**, Thioflavone, 4'-nitro- **422564-16-7**, Thioflavone, 6-methoxy-
(preparation of)

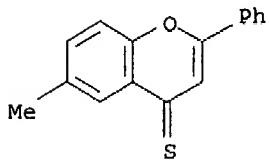
RN 82340-44-1 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



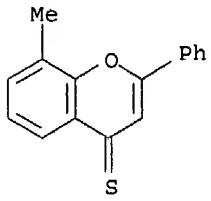
RN 140885-77-4 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



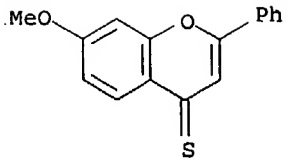
RN 140885-99-0 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 8-methyl-2-phenyl- (9CI) (CA INDEX NAME)

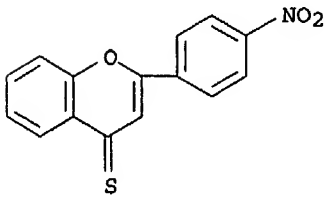


RN 244107-94-6 HCAPLUS

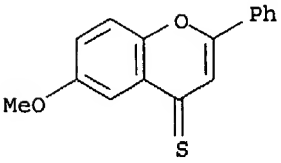
CN 4H-1-Benzopyran-4-thione, 7-methoxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 256464-73-0 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 422564-16-7 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 6-methoxy-2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 58 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:404163 HCAPLUS
DOCUMENT NUMBER: 61:4163
ORIGINAL REFERENCE NO.: 61:635f-h,636a-g
TITLE: Synthesis of quercetylene derivatives
AUTHOR(S): Bayer, Ernst; Kraemer, Bruno
CORPORATE SOURCE: Tech. Hochschule, Karlsruhe, Germany
SOURCE: Ber. (1964), 97(4), 1057-68
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 61:4163

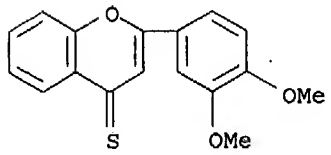
AB The product regarded by Malkin and Nierenstein (CA 24, 4038) as quercetylene (I) is not a dimerization product, but pentaacetoxy-3-flavene (II). The deca-Me ether (III) of I and other 4-biflavenylidenes were prepared from flavanols via the thioflavanols. The biflavenylidenes with the exception of III exhibit piezochromism and piezomagnetism. I (10 g.) in 300 cc. Ac2O refluxed 45 min. with 40 g. Zn dust gave 10 g. II, yellow-red powder, softening at 100-40°. II (10 g.) in 150 cc. 10% HCl-MeOH refluxed 1 hr. gave cyanidine chloride, Rf 0.54, with a compound, Rf 0.75, exhibiting the typical properties of a phlobaphene. 3,4-(MeO)2C6H3COCl (IV) (31 g.) and 12 cc. o-HOC6H4Ac treated dropwise with cooling with 150 cc. dry C5H5N and the mixture heated 1 hr. on the water bath, kept overnight, warmed to 70° to solution, and treated with 20 g. powdered KOH gave the yellow K salt of 3,4-(MeO)2C6H3CO2COAr (V)

(Ar = o-HOC6H4) (VI); the mixture stirred into 500 cc. 10% AcOH precipitated 25 g.
VI, yellow leaflets, m. 129-30° (EtOH). VI (10 g.) boiled briefly with 150 cc. AcOH and 10 cc. concentrated H2SO4 and kept 1 day at room temperature
yielded 7.0 g. 3',4'-dimethoxyflavone, m. 154° (EtOH).
Resacetophenone 4-Me ether (20 g.), 35 g. IV, and 200 cc. dry C5H5N treated with 50 g. KOH, and the K salt of V [Ar = 2,4-HO(MeO)C6H3] (VII) treated with 1 1.10% AcOH yielded 15.5 g. VII, m. 129° (EtOH). VII (15.5 g.) with 200 cc. AcOH and 20 cc. concentrated H2SO4 yielded 3',4,7'-trimethoxyflavone (VIII), m. 178° (EtOH).
Phloracetophenone 2,4-di-Me ether (20 g.), 30 g. IV, and 30 g. KOH in 250 cc. dry C5H5N gave 24 g. V [Ar = 2,4,6-HO(MeO)2C6H2] (IX), yellow leaflets, m. 171-2° (EtOH). IX (24.0 g.) with 100 cc. AcOH and 20 cc. concentrated H2SO4 yielded 10.5 g. 3',4',5,7-tetramethoxyflavone (X), m. 191-2°. Me2NCH2CH2Cl.HCl (20 g.), 15 g. 7-hydroxyflavone, and 1500 cc. dry Me2CO refluxed 72 hrs. with stirring yielded 79% 7-(2-dimethylaminoethoxy)flavone (Xa), needles, m. 121° (petr. ether). The appropriate flavone in MePh-C5H5N treated hot with P2S5 and the mixture refluxed yielded the corresponding 4-thioflavone (XI); in this manner were prepared the following compds. (m.p., color, g.-amount corresponding methoxyflavone used, cc.-volume MePh and C5H5N used, g.-amount P2S5 used, reaction time in hrs., and g.-yield of XI given): 4-thioflavone (XII), 89°, red, 50, 500, 100, 150, 2, 46; 7-MeO derivative (XIII) of XII, 136°, red, 5.5, 100, 20, 15, 4, 4.8; 3',4'-di-MeO derivative (XIV) of XII, 136°, red, 3.0, 100, 20, 10, 2, 2.8; 3',4',7-tri-MeO derivative (XV) of XII, 172°, red, 5.0, 100, 20, 15, 3, 4.2; 3',4',5,7-tetra-MeO derivative (XVI) of XII, 203°, blue, 5.0, 100, 20, 15, 4, 3.9; 3,3',4',5,7-penta-MeO derivative (XVII) of XII, 170°, blue, 10, 200, 20, 20, 5, 9.0. 7-Carbethoxymethoxyflavone (XVIII) (3.45 g.) in 50 cc. dry C5H5N treated at 70° with 10 g. P2S5 in portions and refluxed 1 hr. yielded 2.8 g. 4-thio analog (XIX) of XVIII, red needles, m. 156° (BuOH). Xa (8.0 g.) in 100 cc. dry C5H5N and 16 g. P2S5 refluxed 2 hrs. yielded 7.6 g. 4-thio analog (XX) of Xa.0.5H2O, red needles, m. 123-4° (ligroine, b. 70-90°). XII (10.0 g.) and 60 g. precipitated Cu powder in 500 cc. dry MePh refluxed 7 hrs. with stirring gave 5.1 g. XXI (R = R1 = R2 = R3 = R4 = H), yellow crystals, m. 226°; in similar runs with MeI, the thioflavone and MeI were stirred 5 hrs. at room temperature before the addition of the Cu powder. In this
manner were prepared the following XXI (R, R1, R2, R3, R4, m.p., color, thioflavone used and g.-amount, g.-amount Cu powder, cc.-volume MePh used, reaction time in hrs., and g.-yield of XXI given): MeO, H, H, H, H (XXII), 224°, yellow, XIII, 2.0, 20, 100, 7, 0.70; MeO, MeO, H, H, H (XXIII), 229°, yellow, XIV, 1.0, 10, 100, 7, 0.63; MeO, MeO, MeO, H, H (XXIV), 227°, yellow, XV, 29.3, 20 (9 cc. MeI added) (30), 100 (250), 12 (9), 0.60 (3.3); MeO, MeO, MeO, MeO, H (XXV), 230°, yellow, XVI, 2.4, 20, 100, 46, 0.30; MeO, MeO, MeO, MeO, MeO (XXVI), 235°, bright yellow, XVII, 14.0, 90 (40 cc. MeI added), 250, 46, 2.5; Me2NCH2CH2O, H, H, H, H (XXVII), yellow, 163-4°, XX, 0.50, 5, 100, 17, 0.03; EtO2CCH2O, H, H, H, H, 163°, yellow, XIX, 12.1 (3 cc. MeI added), 50, 250, 20, 6.7. Raney Ni (80 g.) degassed at 300°/0.1 mm., cooled, moistened with MePh, treated with 10.0 g. XX in 150 cc. MePh, and the mixture refluxed 5 hrs. yielded 7.0 g. XXVII, m. 164°. XVI (2.00 g.) and 20 g. Raney Ni in 200 cc. MePh gave similarly 360 mg. XXV. XVII (0.61 g.) in 150 cc. MePh treated 24 hrs. with 5 g. Raney Ni did not give XXVI. The appropriate XXI (200 mg.) in 50 cc. AcOH treated about 1 min. with dry HCl and the mixture diluted with 200 cc. Et2O and refrigerated 2 days gave the corresponding HCl salt:

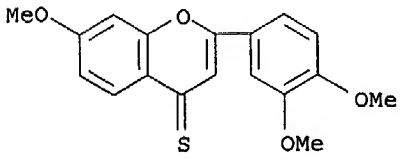
XXII.HCl.H2O, XXIII.HCl.1.1H2O.0.36HCl, XXIV.HCl.3.4H2O.1.9HCl; XXV.HCl.-H2O.1.18HCl, XXVI.HCl.3.9H2O.2.7HCl. XXIV and XXVI were converted by the method of Schoenberg and Asker (CA 36, 41151) to XV, Rf 0.47, and XVII, Rf 0.56. The appropriate bi-flavenylidene (about 20 g.) in 50 cc. refluxing xylene treated 5 hrs. with O yielded VI, Rf 0.46, VIII, Rf 0.40, and 3,3',4',5,7-pentamethoxyflavone, Rf 0.35. 2,4-HO(MeO)C6H3CHO (2.0 g.) and 4.8 g. acetoveratrone in 110 cc. Et2O saturated with cooling with dry HCl, kept 2 days at 5°, saturated again with dry HCl, and kept an addnl. 2 days yielded 2.0 g. 3',4',7-trimethoxyflavylium chloride, m. 133-5°.

IT **93321-88-1**, Flavone, 3',4'-dimethoxy-4-thio- **93876-14-3**, Flavone, 3',4',7-trimethoxy-4-thio- **94303-23-8**, Flavone, 3',4',5,7-tetramethoxy-4-thio- **95279-44-0**, Flavone, 7-[2-(dimethylamino)ethoxy]-4-thio- **98783-15-4**, Acetic acid, [(2-phenyl-4-thioxo-4H-1-benzopyran-7-yl)oxy]-, ethyl ester
(preparation of)

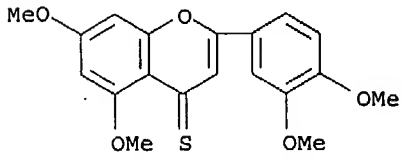
RN 93321-88-1 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



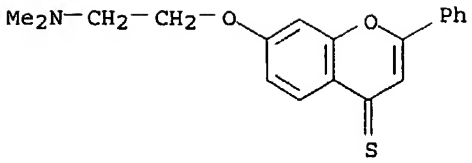
RN 93876-14-3 HCAPLUS
CN Flavone, 3',4',7-trimethoxy-4-thio- (7CI) (CA INDEX NAME)



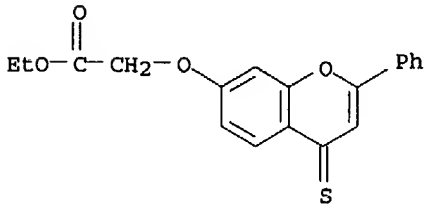
RN 94303-23-8 HCAPLUS
CN Flavone, 3',4',5,7-tetramethoxy-4-thio- (7CI) (CA INDEX NAME)



RN 95279-44-0 HCAPLUS
CN Flavone, 7-[2-(dimethylamino)ethoxy]-4-thio- (7CI) (CA INDEX NAME)



RN 98783-15-4 HCAPLUS
CN Acetic acid, [(2-phenyl-4-thioxo-4H-1-benzopyran-7-yl)oxy]-, ethyl ester (7CI) (CA INDEX NAME)



L32 ANSWER 59 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:52645 HCAPLUS
DOCUMENT NUMBER: 60:52645
ORIGINAL REFERENCE NO.: 60:9236g-h,9237a-h,9238a-e
TITLE: Thiochromones with schistosomicide activity
AUTHOR(S): Bossert, Friedrich; Goennert, Rudolf
SOURCE: Med. Chem., Abhandl. Med.-Chem. Forschungsstaetten Farbwerke Hoechst A. G. (1963), 7, 367-92
DOCUMENT TYPE: Journal
LANGUAGE: German

AB In attempts to find miracil D analogs, the synthesis of some substituted thiochromanones (I) and thiochromones (II) was undertaken. A mixture of 15 g. I(R1 = R2 = H, R3 = NH2, R4 = Me) (m. 86-8°) and 13 g. Et2NCH2CH2Cl was heated 15 min. at 150° to give I [R1 = R2 = H, R3 = Et2N(CH2)2NH, R4 = Me], b0.01 175°. A mixture of I(R1 = H, R2 = R4 = Me, R3 = Cl) (b0.01 151°) (18 g.), 15 mL. Et2N(CH2)2NH2, and 15 mL. C5H5N in the presence of Cu powder was heated 60 h. at 150° in a sealed tube to give I [R1 = H, R2 = R4 = Me, R3 = Et2N(CH2)2NH], b0.01 190°. Similarly were prepared the following I (R4 = Me) (R1, R2, R3, and b.p. given): Me, H, Et2N(CH2)2NH, b0.01 176° (HCl salt m. 175°); Et, H, Et2N(CH2)2NH, b0.01 180°; H, Me, Et2N(CH2)2NH, b0.01 190° (picrate m. 135°); Me, H, N-methylpiperazino, -- (m. 75-7°); H, Me, N-methylpiperazino, b0.01 175°. A mixture of II [(R1R2 =)(CH2)4, R3 = Cl, R4 = Me] (9 g.), 10 mL. (N-methylpiperazino)ethylamine, 9 g. NaHCO3, and 140 mL. xylene was refluxed 60 h. to give II [(R1R2 =)(CH2)4, R3 = β-(N-methylpiperazino)ethylamino, R4 = Me], m. 139-41°. II [(R1R2 =)(CH2)4, R3 = ClCH2CONH, R4 = Me] (15 g.), obtained by refluxing 1 h. a mixture of the free amine and ClCH2COCl in C6H6, and 15 mL. morpholine was refluxed 24 h. in 300 mL. EtOH to give the morpholinoacetamido derivative, m. 216-18°. Similarly prepared were the following II (R4 = Me) (R1, R2, R3, and m.p. given): H, H, NHCH2CH2NEt2, -- (b0.01 174°) (HCl salt m. 164°); Me, H, Et2N(CH2)2NH, 71° (b0.01 205°); (HCl salt m. 196°); Et, H, Et2N(CH2)2NH, -- (b0.01 200°); H, Me, Et2N(CH2)2NH, -- (b0.01 185°); H, MeO, Et2N(CH2)2NH, 86°

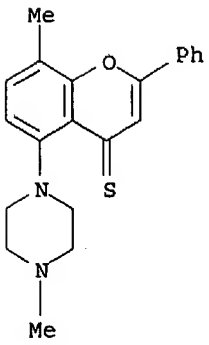
(picrate m. 203°); Me, Me, Et2N(CH2)2NH, 73-5°; Me, Et, Et2N(CH2)2NH, 64-5°; Me, Pr, Et2N(CH2)2NH, 70-2°; Me, iso-Pr, Et2N(CH2)2NH, -- (b0.001 185°); (picrate m. 183-5°); cyclohexyl, H, Et2N(CH2)2NH, -- (b0.01 225°); Ph, H, Et2N(CH2)2NH, -- (HCl salt m. 216-17°); p-MeOC6H4, H, Et2N(CH2)2NH, -- (b0.001 265°); (HCl salt m. 184-6°); p-ClC6H4, H, Et2N(CH2)2NH, -- (b0.001 260°); m-ClC6H4, H, Et2N(CH2)2NH, 92-5°; o-ClC6H4, H, Et2N(CH2)2NH, -- (b0.001 235°); 2-thienyl, H, Et2N(CH2)2NH, 75-7° (HCl salt m. 219-21°); H, Ph, Et2N(CH2)2NH, 102-3°; Me, Ph, Et2N(CH2)2NH, 98-100°; Me, H, N-methylpiperazino, 81-5°; Ph, H, N-methylpiperazino, 134-6°; Me, H, Et2NCH2CONH, 151-3°; Me, H, Bu2NCH2CONH, 49-51°; Me, H, morpholinoacetamido, 177°; Ph, H, Et2NCH2CONH, 115°; (R1R2 =)(CH2)3, Et2N(CH2)2NH, 101-3°; (R1R2 =)CH2CHMeCH2, Et2N(CH2)2NH, 81-3°; (R1R2 =)(CH2)4, Et2N(CH2)2NH, 94-6°; (R1R2 =)CH2CHMeCH2CH2, Et2N(CH2)2NH, 97-9°; (R1R2 =)CH2CH2CHMeCH2, Et2N(CH2)2NH, 75-7°; (R1R2 =)CH2CH2CMe:CH, Et2N(CH2)2NH, 71-3° (HCl salt 171-2°); (R1R2 =)CH2SCH2CH2, Et2N(CH2)2NH, 67° (HCl salt m. 181-2°); (R1R2 =)(CH2)4, β-(N-methylpiperazino)ethylamino, 139-41°; (R1R2 =)(CH2)4, γ-morpholinopropylamino, 95-6°; (R1R2 =)(CH2)4, N-methylpyrazino, 134-6°; (R1R2 =)(CH2)4, thiomorpholino, 135-7°; (R1R2 =)(CH2)4, Et2NCH2CONH, 161-2°; (R1R2 =)(CH2)4, morpholinoacetamido, 216-17°. A mixture of I (R1 = R2 = R3 = H, R4 = CO2H) (42 g.) (m. 220°), 30 mL. Et2NCH2CH2Cl, and 400 mL. iso-PrOH was refluxed 12 h. to precipitate the β-N,N-diethylaminoethyl ester hydrochloride, m. 190° (EtOH-Et2CO). Also prepared were 5-(β-diethylaminoethylamino)-8-methylchromanone, b5 195° (HCl salt m. 190-1°), 3-methoxy-5-(β-diethylaminoethylamino)-8-methylchromone, b0.01 170° (HCl salt m. 221°), 6-chloro-8-(β-diethylaminoethyl)aminothiochromone, b0.001 186°, and 2,3-tetramethylene-6-chloro-8-(β-diethylaminoethyl)aminothiochromone, m. 115-17°. Also prepared were the following II (R1, R2, R3, R4, and m.p. HCl salt given): p-Et2NCH2CH2NHC6H4, H, Et2N(CH2)2NH, Me, -- (base b0.001 260°); Me, H, Et2N(CH2)2NH, Cl, 215-16° (base b0.1 230°); (R1R2 =)(CH2)4, Et2N(CH2)2NH, Cl, 101-2°; H, MeO, H, Et2N(CH2)2NH, 254° (base b0.01 212-15°); Ph, H, H, Et2N(CH2)2NH, 226-7° (base m. 99-100°); (R1R2 =) (CH2)4, N-methylpiperazino, Cl, -- (base m. 164-6°); Ph, H, H, N-methylpiperazinoacetamido, -- (base m. 199-200°); (R1R2 =) (CH2)4, Et2N(CH2)2O2C, Me, 195°; (R1R2 =)(CH2)4, Et2N(CH2)2O2C, Cl, 211-13°; (R1R2 =)(CH2)3, H, Et2N(CH2)2O2C, 242°; (R1R2 =)(CH2)3, H, Me2N(CH2)O2C, 204-6°. Also prepared was 2,3-trimethylene-6-chloro-8-(β-diethylaminoethyl)oxycarbonylchromone, 245°. [2,5-Me(O2N)C6H3]2S2 (III) (m. 150°) was obtained from 118 g. 4-nitrotoluene-2-sulfonyl chloride, 4.2 g. KI, and 2 mL. concentrated HCl in 140 mL. dioxane and 30 mL. H2O with portionwise addition of 124 g. Na2S2O5 at 50°; after addition of 30 mL. H2O the mixture was heated 1 h. at 75-80°. To a suspension of 48 g. III in 150 mL. EtOH at 60° were added 22 g. Na2S in 10 mL. H2O and 12 g. NaOH in 30 mL. H2O, the mixture kept 15 min., 300 mL. hot H2O added, the mixture cooled to 30°, treated with a neutralized solution of 40 g. β-chloropropionic acid in 120 mL. H2O, and refluxed 30 min. to give 2,5-R1R2C6H3SR (IV) (R = CH2CH2CO2H, R1 = Me, R2 = NO2) (V), m. 137-8°. 2-Methyl-5-chlorothiophenol (30 g.) at 80° in the presence of a little NaOMe was treated with 26 mL. Et methacrylate and the mixture heated

30 min. at 80-90° to give IV (R = CH2CHMeCO2Et, R1 = Me, R2 = Cl), b3 156°, which was saponified by 1:1 HCl to the free acid, b3 186°, m. 54-5°. Similarly were prepared the following IV (R, R1, and R2 given): (CH2)3CO2H, Me, NO2, m. 119°; (CH2)4CO2H, Me, NO2, oil; (CH2)2CO2H, Me, Cl, m. 114-15°; (CH2)3CO2H, Me, Cl, b3 185°; (CH2)2CO2H, CO2H, H, m. 195°. Also prepared was β-(2-methyl-5-nitrophenoxy)propionic acid (VI), m. 150° (MeOH-H2O). To 90 g. FeSO4 in 230 mL. H2O at 90-5° a solution of 10 g. V in dilute NH3 was added followed by excess NH3, and the mixture kept 30 min. to give β-(2-methyl-5-aminophenylthio)propionic acid (VII), m. 142°. VI (168 g.) in 500 mL. THF .apprx.2 h. at 60-80° was hydrogenated in the presence of 20 g. Raney Ni to β-(2-methyl-5-aminophenoxy)propionic acid, m. 171°. Similarly were prepared IV [R = (CH2)3CO2H, R1 = Me, R2 = NH2], m. 122°, IV [R = (CH2)2CO2H, R1 = NH2, R2 = H], m. 84°, β-(2-amino-4-chlorophenylthio)propionic acid, m. 89-90°, β(2-chloro-5-aminophenoxy)propionic acid, m. 161-2° (EtOH), and β-(2-methyl-5-aminophenoxy)valeric acid, m. 94° (C6H6). 5-Amino-8-methylthiochromanone (VIII) (m. 86-8°, b4 178°) was prepared by dissolving 100 g. VII in 800 mL. concentrated H2SO4 at 50°, and pouring the dark red solution 30 min. later on ice. Similarly prepared were the following I (R1, R2, R3, and R4 given): Me, H, NH2, Me, m. 76-8°, b4 182°; H, H, H, NH2, m. 102° (EtOH); H, H, Cl, Me, m. 70-2°, b3 166°; Me, H, Cl, Me, b3 163°; H, Me, Cl, Me, b0.01 151°; Et, H, Cl, Me, b3 164-8°. Also prepared were 6-chloro-8-methylthiochromanone, m. 105-7°, 5-amino-8-methylchromanone, m. 85-8°, b4 158°, and 8-nitrochromanone, m. 121° (EtOH). 5-Acetamido-8-methylchromanone (m. 164°) (100 g.) and 100 g. p-nitrosodimethylaniline in 400 mL. EtOH refluxed 5 min. with 100 mL. 1% NaOEt gave 3-hydroxy-5-amino-8-methylchromanone, m. 185° (C6H6); 3-methoxy analog m. 150°. Similarly prepared were the following II (R1 = H) (R2, R3, R4, and m.p. given): OH, NH2, Me, 170°; OMe, NH2, Me, 171°; OH, Cl, Me, 161°; MeO, Cl, Me, 154°; OH, H, NO2, .apprx.210°; MeO, H, NO2, 192°; MeO, H, NH2, 176°. II (R1 = R2 = H, R3 = NH2, R4 = Me), m. 146-8° (C6H6), is obtained by adding 100 g. VIII (100 g.) to a mixture of 500 mL. C5H5N and 100 mL. Ac2O at 5-10°, stirring overnight, precipitating 5-acetamido-8-methylthiochromanone, m. 168-70°, with H2O, adding 48 g. IX portionwise to a solution of 30 g. SO2Cl2 in 100 mL. CH2Cl2, refluxing the mixture 10 min., evaporating, refluxing the residue 30 min. in 200 mL. PhNMe2, adding the mixture to dilute H2SO4, and removing the AcO group with EtOH-HCl. Similarly prepared was 2,8-dimethyl-5-aminothiochromone, m. 172°, via 2,8-dimethyl-5-acetamidothiochromanone, m. 141° (MeOH). Polyphosphoric acid (500 g.) at 90° stirred with dropwise addition of a mixture of 30 mL. 2-methyl-5-chlorothiophenol and 40 mL. Et cyclohexan-1-one-2-carboxylate, and the mixture heated 1 h. at 90-100°, gave 2,3-tetramethylene-5-chloro-8-methylthiochromone, m. 132° (C6H6-ligroine). Similarly prepared were 2,8-dimethyl-5-chlorothiochromone, m. 130° (ligroine), and 2,3-tetramethylene-5-amino-5-methylthiochromone, m. 180° (EtOH), from 2-methyl-5-acetamidothiophenol and cyclohexan-1-one-2-carboxylate. II showed the same regularities between constitution and activity on the Schistosoma mansoni infection of mice as did the thioxanthones.

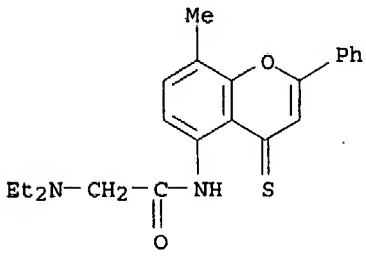
IT **94861-97-9**, Thioflavone, 8-methyl-5-(4-methyl-1-piperazinyl)- **95134-20-6**, Thioflavone, 5-[2-(diethylamino)acetamido]-8-methyl- **95165-24-5**, Thioflavone, 2'-chloro-5-[[2-(diethylamino)ethyl]amino]-8-methyl- **95165-25-6**, Thioflavone, 3'-chloro-5-[[2-(diethylamino)ethyl]amino]-8-methyl- **96266-99-8**, Thioflavone, 4'-chloro-5-[[2-(diethylamino)ethyl]amino]-8-methyl-

97114-61-9, Thioflavone, 5-[[2-(diethylamino)ethyl]amino]-8-methyl-
97155-98-1, Thioflavone, 4',5-bis[[2-(diethylamino)ethyl]amino]-
8-methyl- **97572-10-6**, Thioflavone, 8-[[2-
(diethylamino)ethyl]amino]-
(preparation of)

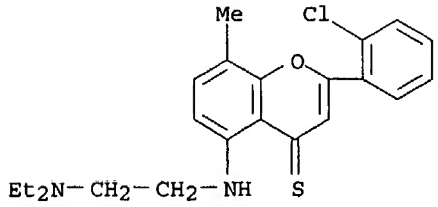
RN 94861-97-9 HCAPLUS
CN Thioflavone, 8-methyl-5-(4-methyl-1-piperazinyl)- (7CI) (CA INDEX NAME)



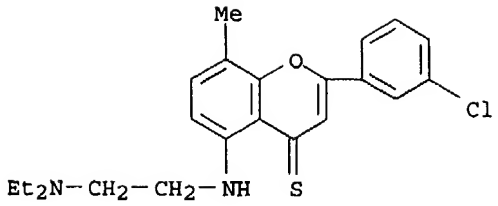
RN 95134-20-6 HCAPLUS
CN Thioflavone, 5-[2-(diethylamino)acetamido]-8-methyl- (7CI) (CA INDEX NAME)



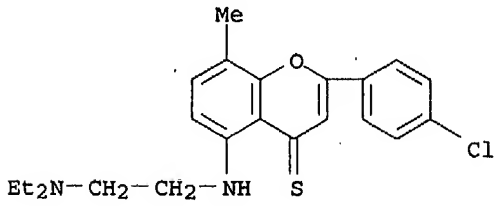
RN 95165-24-5 HCAPLUS
CN Thioflavone, 2'-chloro-5-[[2-(diethylamino)ethyl]amino]-8-methyl- (7CI) (CA INDEX NAME)



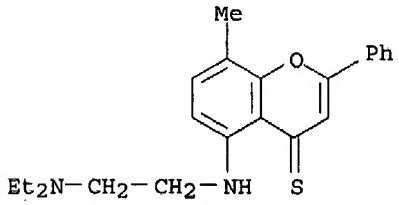
RN 95165-25-6 HCAPLUS
CN Thioflavone, 3'-chloro-5-[[2-(diethylamino)ethyl]amino]-8-methyl- (7CI) (CA INDEX NAME)



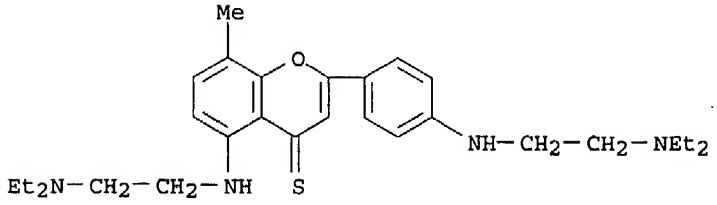
RN 96266-99-8 HCAPLUS
CN Thioflavone, 4'-chloro-5-[[2-(diethylamino)ethyl]amino]-8-methyl- (7CI) (CA INDEX NAME)



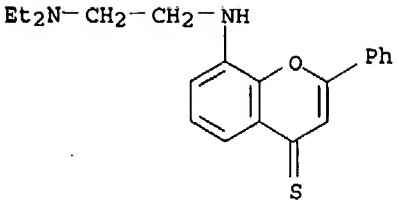
RN 97114-61-9 HCAPLUS
CN Thioflavone, 5-[[2-(diethylamino)ethyl]amino]-8-methyl- (7CI) (CA INDEX NAME)



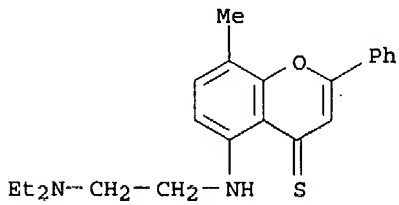
RN 97155-98-1 HCAPLUS
CN Thioflavone, 4',5-bis[[2-(diethylamino)ethyl]amino]-8-methyl- (7CI) (CA INDEX NAME)



RN 97572-10-6 HCAPLUS
CN Thioflavone, 8-[[2-(diethylamino)ethyl]amino]- (7CI) (CA INDEX NAME)



L32 ANSWER 60 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:41588 HCAPLUS
DOCUMENT NUMBER: 60:41588
ORIGINAL REFERENCE NO.: 60:7349a-b
TITLE: Thioxanthones and related compounds in experimental schistosomiasis
AUTHOR(S): Goennert, R.; Koelling, H.
CORPORATE SOURCE: Farbenfabriken Bayer, A.-G., Wuppertal-Eberfeld, Germany
SOURCE: Drugs, Parasites Hosts, Symp., Middlesex Hosp. Med. School (1962) 29-40, discussion 40-2
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Work on xanthones, thioxanthones, thiochromes, toluenes, xylenes, tetrahydroquinolines, and other chemical classes, and the testing of these compds. in mice led to the introduction of lucanthone hydrochloride for the treatment of human schistosomiasis. Lucanthone is the thioxanthone analog of miracil A resulting from the substitution of ring O by S. The results demonstrated that a basic side chain, a Me group para to it, and in some instances, addnl. substituents are prerequisites for schistosomicidal activity in mice. 36 references.
IT **97114-61-9**, Thioflavone, 5-[[2-(diethylamino)ethyl]amino]-8-methyl- (in schistosomiasis treatment)
RN 97114-61-9 HCAPLUS
CN Thioflavone, 5-[[2-(diethylamino)ethyl]amino]-8-methyl- (7CI) (CA INDEX NAME)

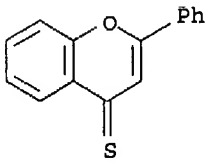


L32 ANSWER 61 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:23264 HCAPLUS
DOCUMENT NUMBER: 60:23264
ORIGINAL REFERENCE NO.: 60:4096h,4097a
TITLE: Benzopyrylium salts. VII. Reaction of flavylium perchlorate with ethyl esters of α-amino acids
AUTHOR(S): Shriner, R. L.; Sutton, Russell

CORPORATE SOURCE: State Univ. Iowa, Iowa City
SOURCE: Journal of the American Chemical Society (1963), 85(24), 3989-91
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 60:23264

AB cf. CA 47, 7496f. Flavylium perchlorate reacted with the Et esters of glycine, alanine, and phenylalanine to form Et N-(2-phenyl-4H-1-benzopyran-4-ylidene)amino acid ester hydroperchlorates, the hydroperchlorate of the amino acid ester, and a mixture of nonnitrogen-containing by-products which have been characterized as 2-hydroxychalcone, 2-phenyl-1,2-benzopyran-2-ol, and 2-phenyl-1,4-benzopyran-4-ol. The degradation of the new substituted benzopyranimines to 4-thioflavone and synthesis from this compound are described.

IT **5465-04-3**, Flavone, 4-thio-
(preparation of)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 62 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1963:408829 HCAPLUS
DOCUMENT NUMBER: 59:8829
ORIGINAL REFERENCE NO.: 59:1577f-h,1578a
TITLE: The action of tetrachloro-o-quinone on thiobenzophenone, 4-thioflavone, and related compounds
AUTHOR(S): Schoenberg, Alexander; Singer, Erich
CORPORATE SOURCE: Tech. Univ., Berlin
SOURCE: Ber. (1963), 96, 1256-8
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 59:8829

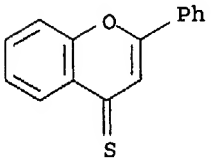
AB Diaryl thio ketones treated with tetrachloro-o-benzoquinone (I) yielded the diaryl methylene ethers of o-C6Cl4(OH)2 (II). 4-Thioflavone (III) and 1,4-dithioflavone (IV) with I yielded 4,5,6,7-tetrachloro-2'-phenyl-(1,3-benzodioxolo-2-spiro-4'-chromene) (V) and the 4'-(1'-thiochromene) analog (VI) of V. Ph2CS (2.1 g.) and 2.40 g. I in 40 cc. dry C6H6 kept 24 hrs. at room temperature, refluxed 1 hr. under N, and evaporated, and the tacky residue ground with a little EtOH gave 2.99 g. 4,5,6,7-tetrachloro-2,2-diphenyl-1,3-benzodioxole (VII), m. 144-5° (EtOH). I (1.23 g.) in 40 cc. dry C6H6 treated at room temperature with 1.5 g. (p-MeOC6H4)2CN2, diluted after 12 hrs. with 60 cc. ligroine (b. 90-100°) and refrigerated yielded 1.87 g. 2,2-bis(p-MeOC6H4) analog (VIII) of VII, lancets, m. 217-19° (BuOH). (p-MeOC6H4)2CS (1.29 g.) and 1.23 g. I in 50 cc. dry C2H6 kept 12 hrs. at room temperature, filtered, and evaporated gave 1.05 g.

VIII. I (2.4 g.) and 2.4 g. III in 100 cc. dry C6H6 or MePh kept 10 hrs. at room temperature and filtered gave the very hygroscopic, yellowish, crystalline V, m. about 280° (decomposition) (dry xylene or MePh). V (0.75 g.) in 30 cc. dioxane and 2 cc. concentrated HCl refluxed 1 hr. under N and evaporated, the residue treated with 30 cc. AcOH and 2 cc. 70% HClO4 and filtered, and the filter residue decomposed with 10% aqueous NaHCO3 yielded 0.27 g. flavone (petr. ether); a similar run added after completion of the hydrolysis to cold, dilute HCl and filtered, and the dried residue refluxed 1 hr. with 30 cc. Ac2O and poured onto ice gave 0.39 g. diacetate (IX) of II. I (2.46 g.) and 2.54 g. IV in 150 cc. dry C6H6 kept 4 hrs. at room temperature, filtered, and evaporated gave 2.60 g. VI, brownish crystals, m. 210-12° with sintering at 200° (decomposition) (ligroine). VI (1.00 g.) in 40 cc. dioxane and 4 cc. concentrated HCl refluxed 1 hr. poured into H2O, and filtered after several hrs., and the residue treated with 40 cc. AcOH and 4 cc. 70% HClO4, filtered, and decomposed with 10% aqueous NaHCO3 yielded 0.42 g. 1-thioflavone; the filtrate added to H2O and filtered, and the residue refluxed 1 hr. with 40 cc. Ac2O and poured onto ice gave 0.43 g. IX.

IT **5465-04-3**, Flavone, 4-thio-
(reaction with tetrachloro-o-quinone)

RN 5465-04-3 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 63 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1955:20054 HCAPLUS

DOCUMENT NUMBER: 49:20054

ORIGINAL REFERENCE NO.: 49:3953f-i,3954a-d

TITLE: Reactions of 4-thiochromones with amino-compounds and with methyl iodide

AUTHOR(S): Baker, Wilson; Clarke, G. G.; Harborne, J. B.

CORPORATE SOURCE: Univ. Bristol, UK

SOURCE: Journal of the Chemical Society, Abstracts (1954) 998-1002
CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

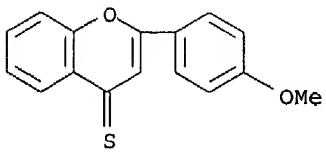
AB (cf. C.A. 47, 1141e). The following 4-thiochromones were prepared by heating the chromones with P2S5 in C6H6 or PhMe for 2 h. and then crystallizing from EtOH: 2-(2-furyl), m. 108°; 2-ethoxycarbonyl, m. 101-3°; and 2,3-di-Ph, m. 175°. Several thioflavones were prepared by rearrangement of the parent flavones in a mixture of powdered KOH in C5H5N. In this manner were prepared the following 4-thioflavones: 4'-methoxy, m. 137°; 7-methoxy, m. 134-6°; 5,7-dimethoxy, m. 184°; 3-Me, m. 128-9°. Also prepared were 2-methyl-4-thioisoflavone, m. 134°; 4-thioisoflavone, m. 94°, and 4-thio-3-flavanol, m. 80-2°. The 4-thiochromones

were heated with 2 equivs. PhCH2NH2 in EtOH 1-2 h., the mixture poured into H2O after the evolution of H2S ceases, and the 4-(benzylimino) derivative isolated (reaction A). Prepared in this manner are the 4-benzylimino derivs. of 2-(2-furyl)-chromone, m. 120-2°, and 4'-methoxyflavone, m. 134.5-5°. 4-Thioisoflavone yielded the benzylimine (I, R = H), m. 109-10.5°; and 2,3-diphenyl-4-thiochromone gave the benzylimine (I, R = Ph), m. 154-5°. N2H4.H2O is added to an alc. solution of the thiochromone, H2S is liberated and the product is isolated after treatment with H2O to yield either a chromone hydrazone or a pyrazole (II). Prepared in this manner are the hydrazones of the following; 2-(2-furyl)-chromone, m. 139-40°; 4'-methoxyflavone, m. 169°; and 7-methoxyflavone, m. 84-94°. Under more drastic conditions, these hydrazones are isomerized to the corresponding IV. Thus, 5,7-dimethoxy-4-thioflavone gave 3(or 5)-(2-hydroxy-4,6-dimethoxyphenyl)-5(or 3)-phenylpyrazole, m. 116-17°; 3-methyl-2-phenyl-4-thiochromone gave 3(or 5)-o-hydroxyphenyl-4-methyl-5(or 3)-phenylpyrazole, m. 138-40°; 2-methyl-3-phenyl-4-thiochromone gave 3(or 5)-o-hydroxyphenyl-5(or 3)-methyl-4-phenylpyrazole, m. 180°; 4-thioisoflavone gave 3(or 5)-o-hydroxyphenyl-4-phenylpyrazole, m. 114-16°; and 2,3-diphenyl-4-thiochromone yielded 3(or 5)-o-hydroxyphenyl-4,5(or 3,4)-diphenylpyrazole, m. 230-1°. The reaction with PhNHNH2 is carried out at 100° for 2-3 h. Thus, 2-(2-furyl)chromone phenylhydrazone, m. 156-8°, was obtained. 4-Thiochromone gave 5-(o-hydroxyphenyl)-1-phenylpyrazole, m. 105-6°; 2-methyl-3-phenyl-4-thiochromone gave 3(or 5)-(o-hydroxyphenyl)-5(or 3)-methyl-1,4-diphenylpyrazole, m. 219-20°. By dissolving the thiochromones in MeI and filtering off the product in 24 h., the methiodides of the following were obtained: 2-(2-furyl)-4-thiochromone, m. 195°; 4'-methoxy-4-thioflavone, m. 206-7°; 7-methoxy-4-thioflavone, m. 210-12°; 5,7-dimethoxy-4-thioflavone, m. 214° (decomposition). In the same manner, the methotriiodides of the following are formed: 2-ethoxycarbonyl-4-thiochromone, m. 166°; 3-methyl-4-thioflavone, m. 99-100°; 4-thiochromone, m. 148-50°. Flavone benzylimine in MeI yielded a methiodide, m. 210-12°.

IT **82340-44-1**, Flavone, 4'-methoxy-4-thio- **84212-80-6**, Flavone, 5,7-dimethoxy-4-thio- **244107-94-6**, Flavone, 7-methoxy-4-thio-
(preparation of)

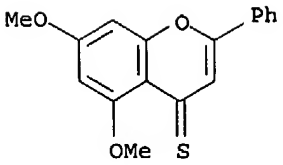
RN 82340-44-1 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

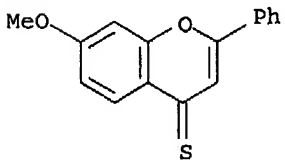


RN 84212-80-6 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 5,7-dimethoxy-2-phenyl- (9CI) (CA INDEX NAME)



RN 244107-94-6 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 7-methoxy-2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 64 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1953:6370 HCAPLUS
DOCUMENT NUMBER: 47:6370
ORIGINAL REFERENCE NO.: 47:1141e-i,1142a-c
TITLE: Some properties of 4-thionflavone and its methiodide and of 4-thionchromones
AUTHOR(S): Baker, Wilson; Harborne, J. B.; Ollis, W. D.
CORPORATE SOURCE: Univ. Bristol, UK
SOURCE: Journal of the Chemical Society, Abstracts (1952) 1303-9
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 47:6370

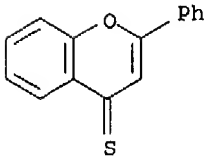
AB Flavone (I) (5 g.), 10 g. purified P2S5, and 50 cc. PhMe, heated 3.5 hrs. on the steam bath, give 55% 4-thioflavone (II), deep red, m. 87°; 250 mg. II, 10 cc. EtOH, and 1 cc. concentrated HCl, heated 40 hrs. on the steam bath, give 65% I. II (300 mg.) and 5 cc. MeI in 15 cc. CHCl3 (18 hrs.) give 96% II methiodide (III), maroon, m. 220-2°; boiled 10 min. with H2O, III yields 92% I. III (250 mg.) and 1 cc. PhNH2 in EtOH, shaken 15 min., give 82% flavone anil, deep yellow, m. 121.5-2.5° [picrate, yellow, m. 230-40° (decomposition)]. II (200 mg.) in 10 cc. warm EtOH, treated with 0.5 cc. N2H4.H2O, and, after 10 min., diluted with H2O, gives 65% flavone hydrazone (IV), deep yellow, m. 136°; benzylidene derivative, yellow, m. 136°; N-Ac derivative, m. 284°. III (200 mg.) and 72 mg. BzNHNH2 in 10 cc. EtOH give 47% flavone benzoylhydrazone (V), yellow, m. 244° (decomposition); V results in 100% yield from IV and BzCl. III (200 mg.), 1 g. H2NNHCONH2.HCl, and 1 g. AcONa, shaken a few min., give 90% flavone semicarbazone, bright yellow, m. 245° (decomposition), brilliant green fluorescence in ultraviolet light; the thiosemicarbazone (97%), deep yellow, m. 234° (decomposition). II (220 mg.), 220 mg. NH2OH.HCl, and 4 cc. C5H5N, heated 30 min. on the steam bath, give 72% flavone oxime (VI), m. 184-6°; III gives 73% VI; VI is unchanged on refluxing 1 hr. with aqueous-alc. 2 N NaOH or overnight with MeOH-Ba(OH)2. o-HOC6H4COCH2Bz (VII) (1.1 g.), 1 cc. N2H4.H2O, and 10 cc. EtOH, refluxed 20 min., give 97% 3(5)-o-hydroxyphenyl-5(3)-phenylpyrazole (VIII), m. 144°, deep green color with aqueous-alc.

FeCl3. The compound which Gulati and Ray (C.A. 30, 8214.4) assumed to be VI is actually 3-(o-hydroxyphenyl)5-phenylisooxazole (Shenoi, et al., C.A. 34, 2817.6). IV (100 mg.) and 161 mg. III in 5 cc. EtOH, 1 hr. at room temperature, give 100% 4-flavyleneazine (IX), orange, m. 298° (decomposition); IX results in 25% yield by passing (2 hrs.) H2S through IV in boiling EtOH. VII (1 g.), 0.44 cc. PhNHNH2, and 10 cc. EtOH, refluxed 2.5 hrs., give 3-o-hydroxyphenyl-1,5-diphenylpyrazole (X), m. 105-6°; flavone phenylhydrazone is not isomerized to X by heating with alkali. Flavone 2,4-dinitrophenylhydrazone, m. 282° (decomposition) (Adkins and Mozingo, C.A. 32, 3399.9), results from 0.5 g. II, 1 g. 2,4-(O2N)2C6H3NHNH2, and 2 cc. H2SO4 in 40 cc. EtOH (8%) or III (79%); it also results from VII in 18% yield. 2-Methylchromone (2.5 g.), 4.8 g. P2S5, and 50 cc. PhMe, refluxed 1.5 hrs., give 56% 2-methyl-4-thiochromone (XI), very deep red, m. 96-7°. XI (200 mg.), 0.24 cc. PhNHNH2, 4 drops 2 N NaOH, and 10 cc. EtOH, refluxed 2 hrs., give 86% 5-o-hydroxyphenyl-3-methyl-1-phenylpyrazole, m. 190-1°; this was also prepared from o-HOC6H4COCH2Ac. 2,3-Dimethyl-4-thiochromone (XII) yields 55% 5-o-hydroxyphenyl-3,4-dimethyl-1-phenylpyrazole, m. 210-11° (Ac derivative, m. 96-7.5°) (Simonis and Rosenberg, C.A. 8, 2385, considered this a phenylhydrazone of XII). XI (250 mg.), 0.5 cc. N2H4.H2O, and 5 cc. H2O, shaken 5 min. at room temperature, give 90% 3(5)-o-hydroxyphenyl-5(3)-methylpyrazole, m. 132-4°, which has also been prepared from o-HOC6H4COCH2Ac (cf. Koenigs and Freund, C.A. 42, 1935h). XII yields 3(5)-o-hydroxyphenyl-4, 5(3,4)-dimethylpyrazole, m. 116-18°, purple-green color with FeCl3. Ultraviolet absorption spectra are given for the pyrazole derivs.

IT **5465-04-3**, Flavone, 4-thio-
(preparation of)

RN 5465-04-3 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 65 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	1947:757 HCAPLUS
DOCUMENT NUMBER:	41:757
ORIGINAL REFERENCE NO.:	41:129a-g
TITLE:	Derivatives of tetrahydroquinoline
AUTHOR(S):	de Diesbach, Henri; Kramer, Hans
CORPORATE SOURCE:	Univ. Fribourg, Switz.
SOURCE:	Helvetica Chimica Acta (1945), 28, 1399-1405 CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE:	Journal
LANGUAGE:	French
OTHER SOURCE(S):	CASREACT 41:757

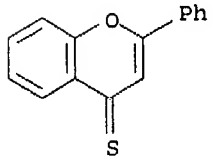
AB A comparative study of certain reactions of flavone (I), flavanone (II), 1-tosyl-4-oxo-1,2,3,4-tetrahydroquinoline (III), and 2-phenyl-III (IV) is made. To 3.5 g. o-NH2C6H4Ac in 5 g. C5H5N is added 5 g. p-MeC6H4SO2Cl and the mixture heated to boiling to give o-tosylaminoacetophenone (V), m. 149° (alc.). V (5 g.) and 2 g. BzH in 50 cc. warm absolute alc., treated to turbidity with EtONa, give the aldol (VI), m. 260°.

Bromination of VI in CHCl3 (warming) gives, after evaporation and crystallization of the residue from alc., o-MeC6H4SO2NHC6H4COCHBrCH(OH)Ph, m. 151°. AcOH and VI give, from alc., yellow 2-tosylaminochalcone(VII), m. 136°. Bromination of VII in CHCl3 gives, from alc., the addition product, m. 140°. VI or VII, in a little warm alc., treated with 5 vols. of warm 1% NaOH, deposits, after long standing, a precipitate of IV, prisms from MeOH or EtOH, m. 138°, in quant. yield. IV-phenylhydrazone, from 0.5 g. IV, 3 g. PhNHNH2 (VIII), and a few drops AcOH (1 hr. on the H2O bath), crystallizes from alc. in brownish-yellow prisms, m. 184°. A mixture of 0.5 g. IV and 0.2 g. BzH in 20 cc. EtOH, saturated with HCl gas (cooling), gives 3-benzylidene-IV (IX), m. 184°. BzH, V, and a few drops piperidine, heated at 150°, yield IX. Addition of 1 mol. equivalent Br to 1 g. IV in 15 cc. CHCl3 (warming), evaporation, and crystallization of the residue from alc. gives 6?-bromo-IV, m. 159°. The Br is not eliminated by C5H5N. PCl5 cyclization of the condensation product of tosylaniline with ClCH2CH2CO2H gives 1-tosyl-4-chloro-1,2-dihydroquinoline and not 3-chloro-III as reported by Clemo and Perkin, C.A. 18, 3382. Addition of 5 cc. of a CHCl3 solution of Br (1 cc. = 0.106 g. Br) to 1 g. III (slight warming), evaporation, and crystallization of the residue from alc. give needles of 3-bromo-III (X), m. 129°. III and double the amount of Br give 3,3-dibromo-III (XI), m. 127°. X or XI in AmOH with Cu powder gives III. On warming with C5H5N, there is elimination of Br accompanied by decomposition II (2.5 g.), 30 cc. alc., and 1.2 g. VIII, boiled for 1 hr. give, from alc., yellow crystals of II-phenylhydrazone, m. 147°. Addition of HCl gas to 1 g. II, 20 cc. alc., and 0.5 g. BzH (cooling) gives, after 1 day, a precipitate of 3-benzylidene-II (XII).HCl, m. 167° (alc.). From the mother liquor XII, m. 105° (MeOH), seps. after some time. II in warm CHCl3, on addition of Br, evaporation, and crystallization of the residue from AcOH, gives 3,3-dibromo-II (XIII), m. 156°. XIII, boiled with 5 times its weight of C5H5N and the mass diluted with H2O and mineral acid, gives, from alc., 3-bromo-I, m. 126°. 4-Thio-I, m. 89° (0.5 g.)(prepared by refluxing for 2 hrs. a mixture of 1 part I, 30 parts C6H6, and 1 part P2S5), 0.5 g. VIII, and 8 g. C5H5N are refluxed together 2 hrs. and the mass diluted with H2O and mineral acid to give, from MeOH, yellow crystals (which become brown in the air) of I-phenylhydrazone (XIV), m. 155°. I and VIII do not give XIV.

IT **5465-04-3**, Flavone, 4-thio-
(preparation of)

RN 5465-04-3 HCAPLUS

CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 66 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN

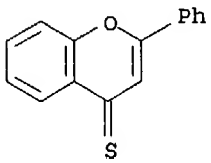
ACCESSION NUMBER: 1942:26830 HCAPLUS

DOCUMENT NUMBER: 36:26830

ORIGINAL REFERENCE NO.: 36:4115a-e
TITLE: Cleavage of the ethylene linkage by the action of sulfur
AUTHOR(S): Schonberg, Alexander; Asker, Waffia
SOURCE: Journal of the Chemical Society, Abstracts (1942) 272-4
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. S., et al., C. A. 20, 364. 1-Thioflavone (1 g.), treated with 15 cc. $SOCl_2$ on a water bath for 10 hrs. and the dark red residue refluxed with 8 g. Cu bronze (I) in 50 cc. C_6H_6 for 6 hrs., gives dithioflavylene (2,2'-di-phenyldithiochromylene) (II), yellow, m. 285°; it gives an orange CCl_4 solution and a yellow H_2SO_4 solution II in glacial AcOH is recovered unchanged after 6 hrs.' refluxing with H_2O and concentrated HCl (equal vols.). If the dark red oil is refluxed with 4 g. I in 60 cc. C_6H_6 for 6 hrs., there results the compound $C_{30}H_{20}Cl_2S_2$, pale brown, m. 120°; further refluxing with I gives II. Heating 0.5 g. each of II and S at 270-80° gives dithioflavone. α,α'-Diphenyl-γ-thiopyrone (III) with $SOCl_2$, followed by refluxing with I in C_6H_6 for 7 hrs. gives, α,α',α'',α'''-tetraphenyl-γ,γ'-dithiopyrylene (IV), dark green, m. about 300° (decomposition); this does not react with S at about 200°. The β-Cl derivative of III gives the β,β'-di-Cl derivative of IV, reddish brown, m. 282-4°. Refluxing 15 g. xanthone with $SOCl_2$ for 8 hrs. and the oil with I in xylene for 10 hrs. gives 9.4 g. of dixanthylene (V), greenish yellow, m. 307°. Heating equal wts. of V and S at 300° for 1 min. gives a dark green liquid. Thioxanthone (5 g.) gives 3.4 g. of dithioxanthylene (VI), m. above 350°; the needles show a blue fluorescence in the solid state and in cold C_6H_6; the cold solution in o-$C_6H_4(CO_2Et)_2$ also shows a blue fluorescence, which diminishes rapidly on heating. Heating 1 g. VI and 0.5 g. S at 260-70° for 0.5 hr. gives thioxanthione. Diflavylene (VII) and S at 290° for 1 hr. give 4-thioflavone. VI and II are changed only very slightly or not at all when air is passed through their C_6H_6 solns. for 10 hrs. at room temperature VII but not II gives, when pressed in a mortar, a dark red color which changes to yellow on addition of a drop of ether. An explanation of the S cleavage reaction is given.

IT **5465-04-3**, Flavone, 4-thio-
(preparation of)
RN 5465-04-3 HCAPLUS
CN 4H-1-Benzopyran-4-thione, 2-phenyl- (9CI) (CA INDEX NAME)



L32 ANSWER 67 OF 67 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1914:7414 HCAPLUS
DOCUMENT NUMBER: 8:7414
ORIGINAL REFERENCE NO.: 8:1118a-d

TITLE: Naphthoflavones and naphthathioflavones
AUTHOR(S): Ruhemann, Siegfried
CORPORATE SOURCE: Univ. Cambridge
SOURCE: Ber. (1914), 47, 119-25
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C. A., 8, 348. Like the phenols and thiophenols, so also the naphthols and thionaphthols (in the form of their Na salts) combine with PhC:CCO2R to form β-naphthoxy- and β-naphthylthiocinnamic esters which are easily converted into the flavones and thioflavones. The Na naphtholates and thionaphtholates are difficult to obtain pure, however, and the yield of substituted PhCH:CHCO2R is less satisfactory than in the case of the C6H6 derivs. α-Naphthoflavone (Kostanecki, Ber., 31, 707) was obtained in this way from α-C10H7OCPh:CHCO2H, PCl3 and AlCl3 in C6H6 suspension. Ethyl β-[β-naphthoxy]chinnamate, obtained in 30% yield from β-C10H7ONa suspended in PhMe and PhC:CCO2Et after 1 hr. heating, reddish oil, b23 285-90°, leaflets, m. 161-2°, gives with alc.KOH a red color turning to yellow on heating and yielding after b. 1 hr. the free acid, needles, m. 164° (loss of CO2), converted by PCl5 and AlCl3 in C6H6 into β-naphthoflavone, needles, m. 164-5°, soluble without color but with intense blue fluorescence in conc.H2SO4. Ethyl β-[α-naphthylthio]cinnamate, yellowish brown oil, b12 278-80°. Free acid, needles, m. 183-4° (foaming). Thioflavone, leaflets, m. 182°, soluble with yellow color and faint green fluorescence in H2SO4. Ethyl β-[β-naphthylthio]cinnamate, needles, m. 102-3°; yield, 50-60%. Free acid, yellowish prisms, m. 165-6° (foaming), loses CO2 when heated in vacuo, forming the styrene, light yellow oil, b12 238-9°, yellow needles, m. 84-5°. Thioflavone, needles, m. 155°, soluble with yellow color and faint greenish fluorescence in H2SO4.